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NUMERICAL SIMULATION OF GROUND WATER CONTAMINANT TRANSPORT ON A SUPERCOMPUTER WITH INJECTION-PUMPING NETWORKS USING THE MODIFIED MOC AND MFE METHOD

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ON A SUPERCOMPUTER WITH INJECTION-PUMPING NETWORKS
USING THE MODIFIED MOC AND MFE METHOD

BY

CHEN YU CHIANG

A THESIS SUBMITTED
IN PARTIAL FULFILLMENT OF THE
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DOCTOR OF PHILOSOPHY

APPROVED, THESIS COMMITTEE:

P.B. Bedient
P.B. Bedient, Associate Professor
of Environmental Engineering
Chairman

M.F. Wheeler
M.F. Wheeler, Professor
of Mathematical Science
Co-Chairman

J.F. Andrews
J.F. Andrews, Professor
of Environmental Engineering

Houston, Texas
October, 1985
ABSTRACT

To prevent the deterioration of groundwater quality, mathematical simulation models have been formulated to predict the transport of contaminants in complex aquifer systems and to design remedial schemes for the problems.

Existing analytical and numerical approaches have serious disadvantages for large-scale nonhomogeneous field problems where well-pumping or injection is involved. The major difficulties relate to numerical dispersion and oscillations in highly advective-dominated simulations, computational accuracy, excessive computer expense, grid orientation problems, and an inability for simulating with random conductivity fields.

Recent work by Ewing, Russell, and Wheeler (1983) has produced a very efficient and accurate method for miscible displacement in oil reservoirs. Their concept was adapted and then applied to groundwater contaminant transport problems in this thesis. The highly efficient code combines a mixed finite element procedure for groundwater flow and a modified method of characteristics and finite element procedure (MMOC) for the parabolic transport equation. The preconditioned conjugate gradient method was used to solve the resulting matrices for both equations.

The method has been compared with two analytical solutions on a homogeneous domain. Excellent agreements were
demonstrated through relative concentration contours and breakthrough curves. The method has also been compared with the currently popular USGS Solute Transport model. More accurate resolutions were achieved for the MMOC method than for the USGS Solute Transport model. In addition, much larger time steps were allowed in the MMOC method than the USGS Solute Transport model obtaining similar resolutions.

The method has been applied to highly advective-dominated problems on a CRAY-XMP supercomputer and the results showed there are no dispersion or oscillation problems common in many existing numerical codes. The method has also been used to simulate cases with random hydraulic conductivity fields that were simulated from Turning Bands Method. Fingering phenomena developed because the concentration front is transported more rapidly in the zones of higher hydraulic conductivity. The method has been shown to be superior in many respects to currently used models in groundwater transport, especially in the presence of strong pumping or injection centers or heterogeneities in the flow field.
ACKNOWLEDGEMENTS

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NUMERICAL SIMULATION OF GROUNDWATER CONTAMINANT TRANSPORT ON A SUPERCOMPUTER WITH INJECTION-PUMPING NETWORKS USING THE MODIFIED MOC AND MPE METHODS

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CHAPTER ONE

INTRODUCTION

Increased interest in the use of groundwater resources and in the study of groundwater contamination have been seen in recent years. To control the deterioration of groundwater quality, it has become necessary to develop a methodology for monitoring, analyzing, and predicting the movement of contaminants through the subsurface. Mathematical models have been formulated as predictive tools to simulate the transport of contaminants through groundwater systems. Input requirements usually include a description of the hydraulics and pollutant transport mechanisms as well as a description of biotic/abiotic reactions within the environment of the porous media. Analytical methods can provide accurate solutions, but are generally applicable only to idealized homogeneous groundwater systems. Since analytical techniques cannot treat general, nonhomogeneous, large scale groundwater problems, numerical simulation must be considered.

Recent work by Ewing, Russell, and Wheeler (1983) has developed a very efficient and accurate method for modeling incompressible miscible displacement in porous media. The highly efficient method combines a mixed finite element procedure for groundwater flow and a modified method of characteristics and finite element procedure (MMOC) for the parabolic transport equation. The preconditioned conjugate
gradient method is used to solve the resulting matrices for both equations. The modified method of characteristics procedure takes time steps in the direction of flow, along the characteristics of the velocity field of the total fluid. The physical diffusion and dispersion terms are treated by a standard finite element scheme. The mixed finite element procedure involves solving for both pressure and velocities simultaneously.

Mathematical descriptions of groundwater contaminant transport and miscible displacement in porous media are very similar. This research will apply and extend the modified method of characteristics and mixed finite element concepts to general problems of groundwater contaminant transport. The overall objectives of the thesis are:

I. Theory

1. To develop a general groundwater contaminant transport simulator based on Modified Method of Characteristics and Mixed Finite Element Method. This flexibility allows one to design injection-pumping networks for remedial plans to clean up a contaminated field site.

2. To incorporate different boundary conditions into the MMOC method. The purpose for different types of boundary conditions is to increase the code's flexibility to handle more general practical problems.

II. Applications

1. To test the code's accuracy against two analytical solutions. One involves a single injection well and the other involves an injection pumping well pair.
2. To compare the MMOC method with the currently popular USGS Solute Transport model in terms of the solution's accuracy and the code's efficiency.

3. To evaluate the limits of the time step size in the modified method of characteristics.

4. To evaluate the grid size convergence study.

5. To apply the code to simulate cases with highly advective-dominated flow fields.

6. To apply the code to simulate cases with random hydraulic conductivity fields which are simulated from the Turning Bands Method.

Following this chapter is a literature review, which covers dispersion processes, groundwater, common analytical and numerical methods, and applications to field studies. Chapter Three gives a fairly complete treatment of methodology for both hydraulic and transport equations. Chapter Four compares the MMOC method with analytical solutions and the USGS Solute Transport Model. Convergence studies and nonhomogeneous field simulations are also included in this chapter. Chapter Five discusses some results and conclusions.
CHAPTER TWO

LITERATURE SURVEY

Groundwater contaminant transport is governed by complex physical, chemical, and biological processes that affect solute concentration in the ground. These processes include advection, dispersion, adsorption and chemical reactions. The process by which solutes are transported by the bulk motion of flowing groundwater is known as advection (Freeze and Cherry 1979). If advection were the only transport mechanism operative, nonreactive solutes being transported by the fluid would move as a plug. There is a tendency, however, for the solute to spread out from the expected advective path of the flow system. This spreading causes mixing with uncontaminated groundwater and will be of particular concern when toxic or hazardous wastes are involved.

In addition to the spreading, the movement of contaminants in groundwater is affected also by the chemical attenuation that causes transfer of contaminant mass between the liquid and solid phases.

The state of the art approach for the prediction of the behavior of groundwater contaminant transport is to summarize these complex processes in the advection-dispersion equation. For illustration purposes, the one-dimensional advection-dispersion equation that includes chemical attenuation is given as (Freeze and Cherry, 1979):

...
\[
\frac{\partial c}{\partial t} = D_{\alpha} \frac{\partial^2 c}{\partial \alpha^2} - \bar{V}_{\alpha} \frac{\partial c}{\partial \alpha}
\]  

(2.0)

where \(\bar{V}_{\alpha}\) is the average linear groundwater velocity, \(D_{\alpha}\) is the coefficient of hydrodynamic dispersion in the direction of flow, \(c\) is the solute concentration, and \(R_d\) is the chemical attenuation factor. The coefficient of hydrodynamic dispersion can be expressed in terms of two components.

\[D_{\alpha} = \alpha_{\alpha} \bar{V} + D^*\]

where \(\alpha_{\alpha}\) is known as dispersivity and \(D^*\) is the coefficient of molecular diffusion.

There are two main approaches that are commonly used for solving the advection-dispersion equation. The first approach is to use analytical techniques that are limited to constant coefficients and simple geometries, while the second approach is to approximate the solution numerically that allows simulating more complex physical and chemical processes. This chapter will review in depth and in sequence the dispersion process, the adsorption process, analytical solutions, commonly used numerical techniques for solving the advection-dispersion equation, and contaminated field studies.
2.1 SOLUTE TRANSPORT BY MIXING PROCESSES

2.1.1 Diffusion Processes

Spreading or mixing processes include diffusion and mechanical dispersion. Diffusion is fairly well understood and it is modeled as a Fickian process. Mechanical dispersion, on the other hand, is less well understood and appropriate models for field scale dispersion remain in question. The hydrodynamic dispersion includes the effects of molecular diffusion and mechanical dispersion. Prior to the discussion of the mechanical dispersion, it is fruitful to briefly review the Fickian's process.

Diffusion may result from molecular action only, analogous to pure conduction in a heat-transfer process. Fick's law for molecular diffusion can be written as

\[ J = -D \cdot \nabla c \]  \hspace{1cm} (2.1)

where \( J \) is the mass flux of a solute, \( D \) is the coefficient of molecular diffusion, and \( c \) is the concentration of a solute. Eq. 2.1 states the mass of diffusion substance passing through a given cross section is proportional to the concentration gradient. Eq. 2.1 is one form of Fick's law, which is analogous to Fourier's law for thermal conduction which states the proportionality between the rate of heat flow across an isothermal surface and the temperature gradient at the surface. The negative sign of Eq. 2.1 reflects the physical fact that the mass flux from high
concentration to low concentration and the sign of the gradient is opposite that of the mass flux. Small molecules have larger average velocities and lower collision rate than do larger molecules. The higher the temperature, the greater the average velocity. The coefficient of molecular diffusion increases with increases in temperature and decreases with increases in the molecular weight and the size of the individual molecule.

2.1.2 Mechanical Dispersion

Mechanical dispersion is caused by both microscopic and macroscopic effects. Mechanical dispersion on a microscopic scale is a result of deviations of velocity on a microscale from the average groundwater velocity. The deviations of velocity are caused by three mechanisms (Freeze and Cherry, 1979): the drag exerted on the fluid molecules by the roughness of the pore surfaces, the difference in pore sizes along the flow paths followed by the water molecules, and the interfingerling of pore channels. Mechanical dispersion on a macroscopic scale is caused by the presence of large scale heterogeneities within the subsurface (Figure 2.1).

Considerable progress in the past twenty years has been evident in describing and understanding the dispersion process on microscopic scale. Much of this work is based on laboratory studies in small columns.
(Slichter 1905; Harleman and Rumer, 1963; List and Brooks, 1967; Bear, 1961b; Lawson and Elrick 1972; Reynolds, 1978; Shamir and Harleman, 1966). Serious difficulties have arisen in trying to scale up the experimental value (dispersivity values of $10^{-2}$ to 1 cm.) to much larger geologic systems. At larger scales, it is likely that a greater number of heterogeneities will be encountered, and a higher dispersion would be expected (Anderson, 1979). Field measured dispersivity values (in the range of 10 to 100 m) to be several orders of magnitude larger than those indicated by laboratory tests with similar materials (Fried, 1975; Bredehoeft and Pinder, 1973; Konikow and Bredehoeft, 1974). In addition, the magnitude of the dispersion coefficient measured in the field seems to increase with the scale of the experiment.

Within the last six years there have been many attempts at understanding the so-called scale problem of dispersion. Pioneering theoretical work on dispersion was done by Taylor (1953) and Aris (1956). They have shown that when a solute in low concentration is injected in a liquid through an infinite straight capillary of uniform cross-section with a steady convective velocity, then the concentration along the capillary is asymptotically Gaussian. This finding implies that the dispersion is a Fickian process, which implies the variance of the concentration distribution should increase linearly with time or distance, and the
longitudinal dispersion coefficient and the dispersity will be a constant for a constant velocity. An analysis of the variance of the concentration by Sudicky and Cherry (1979) from a field tracer test, indicated that the growth of the variance was nonlinear and the dispersivity increased with distance. A more recent natural-gradient tracer test by Sudicky et. al., (1983) indicated that dispersity values increase along the path of migration. The field analyses indicates that dispersion is not Fickian within the distance which the measurements were taken.

Much of the recent research have been focused on the heterogeneity of the subsurface and the pore-grain system of the porous medium. The randomness of the geometry of the pore-grain system suggested the application of statistical methods for the description of the porous media. Among others, de Josselin de Jong (1958), found that the spreading of the tracer from a point injection in a uniform, two-dimensional field of flow takes approximately the form of a bivariate normal distribution. This resulting distribution depends upon a constant dispersion of the porous medium, which is inconsistent with the more recent findings from field tracer tests (Lee et. al., 1980; Pickens and Grisak, 1981a, 1981b).
2.1.3 The Tensor Form of the Dispersion

Based on the variance of the bivariate distribution of the concentration distribution, Bear (1961) showed that for an isotropic porous media the constant dispersion is a fourth-rank tensor. A physical quantity which is said to be a tensor of a certain rank is characterized by the way it behaves under a change in the coordinate system. Because the groundwater flow equation must be valid in any cartesian coordinate system, the dispersion is also required to be invariant under arbitrary rotation of the coordinates, therefore, the dispersion must be treated as a tensor (Scheidegger, 1961). Formulas and graphical representation are available for this purpose. A common graphical representation for a second-rank symmetric tensor is an ellipse. The second-rank tensor representation of dispersion, described by Scheidegger (1961), is a more traditional and widely accepted approach where:

$$ D_{ij} = \alpha_{ijmn} \frac{V_m V_n}{|V|} $$  \hspace{1cm} (2.2)

where $\alpha_{ijmn} =$ dispersivity of the porous medium

$V_m, V_n =$ velocity in m and n directions respectively

In an isotropic medium and a uniform flow field with average velocity $V$, the second-rank tensor reduces to:

$$ D_L = \alpha_L V $$

$$ D_T = \alpha_T V $$
where the subscripts L and T refer to the longitudinal and transverse dispersion coefficients, D, and dispersivities, \( \alpha \), respectively. In the field applications, one usually is able to measure the dispersivities only in the longitudinal and transverse directions versus the tensor representation in mathematics.

2.1.4 Stochastic Analyses of Dispersion

Recognizing the heterogeneities in the hydraulic conductivity, the scale-dependent dispersion has been related to hydraulic conductivity through stochastic analyses in more recent research activities. Mercado (1967) was the first one to quantify the spatial variation in dispersion as a function of hydraulic conductivity using a statistical analysis. In Mercado's paper (1967), two assumptions were made, the first assumption was that the heterogeneity of natural aquifer is caused mainly by the horizontal stratification of layers having a certain range of permeability; second he assumed that the permeability is normally distributed over the vertical cross-section. Based on these two assumptions, Mercado (1967) demonstrated that the concentration can be represented by the complementary error function. The standard deviation of the concentration distribution \( \sigma_c \), was related to the standard deviation of the hydraulic conductivity \( \sigma_k \) by:

\[
\sigma_c = (\sigma_k / \overline{k}) \overline{x} = (\sigma_k / \overline{k}) Ut
\]  

(2.3)
where $\overline{K}$ is the average permeability of the cross-section, $\overline{X}$ is the mean displacement, and $U$ is the mean velocity.

Fischer (1973) showed that a dispersion coefficient can be defined in terms of the rate of change of variance as

$$\frac{3 \sigma_C^2}{\partial t} = 2D = 2(\sigma_K/\overline{K})^2 \overline{X}U$$  \hspace{1cm} (2.4)

Eq. 2.4 implies that the dipsersivity $\alpha$ can be expressed in terms of the mean displacement $\overline{X}$ as

$$\alpha = (\sigma_K/\overline{K})^2 \overline{X}$$  \hspace{1cm} (2.5)

Eq. 2.5 indicates that the dispersivity increases linearly with the distance traveled. Thus the dispersion process was non-Fickian according to Mercado's (1967) analysis. In addition, if dispersion is a Fickian process, the standard deviation of the concentration distribution would increase with the square root of the distance traveled. According to Eq. 2.3, the standard deviation, $\sigma_C$, grows linearly with the distance of displacement.

Schwartz (1977) demonstrated that the macroscopic scale dispersion is influenced directly by the field hydraulic conductivity distribution based on a probability analysis in a one-dimensional flow system. Schwartz (1977) concluded that the magnitude of the dispersion increases with the variance of the hydraulic conductivity within a porous medium. In addition, the dispersion coefficient is not uniquely defined and could not be considered as a characteristic parameter for some porous media. Following
Schwartz (1977), Smith and Schwartz (1980) used a first-
order nearest-neighbor stochastic process to generate a two-
dimensional hydraulic conductivity field in the so-called
"hybrid deterministic probabilistic" (HDP) model. The HDP
model was combined with the Monte Carlo technique to form
estimates of the probability distribution on the model
output. Analysis of a variety of hypothetical media, based
on the HDP model, showed that the microscopic (column scale)
dispersion theories cannot be simply scaled up to field-
scale situations. One rather surprising finding by Smith
and Schwartz (1980) was that even when large amounts of
statistical information are available about porous media,
there maybe considerable uncertainty in predicting
concentration distributions.

It is clear that the dispersion process is non-Fickian
according to Mercado (1967), Schwartz (1977), and Smith and
Schwartz (1980). However, Bear (1972) showed, on the basis
of central limit theorem, that if the travel time for an
individual tracer particle becomes much larger than the time
interval during which its successive velocities are still
correlated, the dispersion can be represented as a Fickian
process. This means that the Fickian process is valid if
the groundwater system is long enough to provide sufficient
spatial averaging.
2.1.5 Taylor Limit

A procedure for predicting the distance of this initial development period has not yet been perfected. This distance is known as the Fickian limit (also known as the Taylor limit) in the groundwater literature. Gelhar and Axness (1981) and Smith and Schwartz (1980) suggested that the Taylor limit will not be reached until the contaminant has traveled on the order of tens or hundreds of meters from the source. According to a theoretical analysis by Dagan (1982), this distance was approximately equal to 50 L, where L is the integral scale of the natural logarithm of the hydraulic conductivity. Mathematically, L is defined as

\[ L = \int_{0}^{L_Y} \rho_Y(\lambda) \, d\lambda \]

where \( L_Y \) is the range of \( \rho_Y(x) \), and \( \rho_Y \) is the autocorrelation of the hydraulic conductivity. \( L \) may be hundreds to thousands of meters for two-dimensional flow fields. If the Taylor limit is reached at large travel distances then a constant dispersivity value can be evaluated theoretically. Therefore the standard form of the advection-dispersion equation should still be valid after the Taylor limit. Gelhar et. al. (1979) and Gelhar and Axness (1983) derived a variety of expressions for evaluating this asymptotic dispersivity value. Gelhar et. al. (1979) represented the one-dimensional flow and mass transport processes for a perfectly stratified aquifer.
through stochastic equations, using a fourth-order partial differential equation. Using a spectral analysis, the stochastic partial differential equation yielded an explicit expression for the macroscopic longitudinal dispersion coefficient in terms of statistical properties of the hydraulic conductivity. The asymptotic value for the longitudinal dispersivity was \( \alpha_L + \lambda_\infty \) where

\[
\lambda_\infty = \frac{1}{3} \frac{\sigma_K^2 \lambda^2}{\overline{k}^2 \alpha_T}
\]

where \( \sigma_K \) is the standard deviation of the lognormal hydraulic conductivity distribution; \( \lambda \) is a correlation length, \( \overline{k} \) is the mean hydraulic conductivity, and \( \alpha_L, \alpha_T \) are average local longitudinal and transverse dispersivities respectively. Notice that the above derivation was based on the simplifying assumption of perfect stratification in a two dimensional, statistical isotropic medium. Important features were lost when the flow is considered to be two dimensional.

Gelhar and Axness (1983) analyzed the macroscopic dispersion coefficient in a three-dimensional statistically anisotropic heterogeneity with mean flow arbitrarily oriented with respect to the stratification. With an arbitrarily oriented anisotropic conductivity covariance, they confirmed that the macroscopic dispersivity is a second rank tensor and the simple Fickian transport will be valid only after a substantial displacement distance. An
interesting argument about the dimensionality by Gelhar and Axness (1983) is worth noting here. They argued that the more complex but more realistic three-dimensional description yields simple behavior, while constraining the flow to one or two dimensions creates complications of debatable significance. The three-dimensional analysis yields a finite asymptotic longitudinal dispersivity using simple monotonic covariance functions, while a finite asymptotic dispersivity exists only for restricted forms of the conductivity covariance function in the two-dimensional analysis by Gelhar et. al. (1979).

2.1.6 Advection-Diffusion Model

Gillham et. al. (1984) developed an advection-diffusion model, to explain the scale-dependent dispersivity. For a perfectly stratified, layered aquifer system, the advection-diffusion model treats only advection along the direction of flow which is parallel to the bedding. The mixing between high permeability layers and low permeability layers is through the molecular diffusion due to the concentration gradient between stratified layers. Through this mixing process there is an increasing degree of smoothing of vertical concentration profiles (Figure 2.2) Gillham et. al. (1984) attributed this transverse molecular diffusion between layers to be the sole mechanism causing significant longitudinal spreading of a tracer.
FIGURE 2.2 Schematic Representation of the Advection-Dispersion Process
(from Gillham et. al., 1984)
FIGURE 2.3  Concentration Profiles from the Advection-Diffusion Model  
(from Gillham et. al., 1984)
Figure 2.3 shows representative relative-concentration profiles along the longitudinal direction downstream from a finite pulse injection. In this figure, the initial sharp front is gradually transported into a smooth, spread-out and skewed distribution. The longitudinal extent of spreading of the tracer zone increases with time.

Results from the above studies suggested that dispersion is non-Fickian near the source of the contaminant and therefore the standard form of the advection-dispersion equation does not apply. Matheron and Demarsily (1980) and Pickens and Grisak (1981) suggested, using the standard form of the advection-dispersion equation with an equivalent dispersivity, a time dependent function for a point source with a pulse injection. However, Matheron and Demarsily (1980) cautioned that using a time dependent dispersivity is only an artifact and

"...a better mathematical formulation of the transport process in porous media and fractured media, valid for all time, seems necessary."

Until a convincing mathematical formulation of the groundwater solute transport process becomes available, or the non-Fickian-type spreading mechanism is better understood from more field data analysis, the traditional advection-dispersion equation will most probably remain the chief tool for groundwater contaminant transport analyses in the coming years. However, the advection-diffusion "layered" model with slow diffusion into low permeability layer within the porous medium, which is a recently active
research direction, has some promising potentials to
describe the transport of organic solutes.

2.2 ADSORPTION PROCESS

Subsurface solute transport is greatly affected and
altered by chemical attenuation in addition to the
dispersion process. The major chemical process thought to
affect organic contaminants is adsorption. Adsorption is
commonly described as a partition of hydrophobic organics
between the polar aqueous phase and the non-polar solid
phase organics. Numerous laboratory studies (Lambert
1966, 1967, 1968; Hance 1969; Briggs 1969) have shown a strong
correlation between the soil organic carbon, the compound
solubility, and the ratio of the adsorbed to soluble organic
contaminant. A partition coefficient for the adsorption
process can be defined as the concentration in the soil
phase divided by the concentration in the aqueous phase.
The commonly used linear equation for this mechanism is
given by the retardation equation

\[ R = 1 + \frac{\rho_b}{n} K_p \]  \hspace{1cm} (2.7)

where \( \rho_b \) is the bulk density of an aquifer, \( n \) is the
porosity, and \( K_p \) is the partition coefficient. \( K_p \) can be
defined as the mass of solute in the soil phase, \( S \), divided
by the concentration of solute, \( C \), in the aqueous phase.
It is important to recognize that Eq. 2.7 is based on the assumption that equilibrium conditions exist between the solution-phase and solid-phase concentration. Eq. 2.7 is valid only if the reactions are fast relative to the groundwater velocity and if the reactions are reversible, and with a linear relationship between $S$ and $C$, also referred to as a linear isotherm. It has been determined by several researchers (Karickhoff et. al., 1979; Hassett et. al., 1980; Chou et. al., 1982) that the linear isotherm is valid for hydrophobic compound with concentration below $10^{-5}$ molar or less than $1/2$ the compound's solubility in water. Several others investigators (O'Connor and Connolly, 1980; Voice, 1982; Weber et. al., 1982) have noted that the linear isotherm is not valid over a large range of equilibrium concentration for many compounds. There are many other nonlinear functional forms of adsorption isotherms, a large number of which are described by Weber (1972). Among all the functional forms, the Freundlich isotherm is a widely used form to fit laboratory tests and field site measurements. The functional representation for the Freundlich isotherm is

$$S = KC^a$$

(2.8)

where $K_p$ and $a$ are empirical coefficients, if $a=1$, the isotherm is linear, then $K = K_p$. The other commonly used non-linear isotherm is the Langmuir isotherm. The Langmuir isotherm has the form
\[
\frac{1}{S} = \frac{1}{\bar{S}} + \frac{1}{bS_c}
\]

where \(\bar{S}\) is the limiting concentration of solute adsorbed on the solid phase and \(b\) is an enthalpy-related sorption constant. Graphically, the Langmuir and the Freundlich isotherms have the form shown in Figure 2.4 (Weber, 1972). The term \(S\) on the ordinate denotes that amount of the substance that has moved across the solid phase. The conceptual basis and underlying assumptions for each of these nonlinear isotherms have been discussed in detail by Weber (1972).

If \(K_{OC}\) is defined as:
\[K_{OC} = \frac{K_p}{OC}\]

where \(OC\) is the fractional mass of organic carbon in the soil, then the value of \(K_{OC}\) is dependent on particular sizes of the soil, starting with a low \(K_{OC}\) value for the sand, increasing to a maximum in the fine silt (Karickhoff et al., 1979). Using a linear least-squares fitting, Karickhoff et al. (1979) related the \(K_{OC}\) value to the octonal/water partition coefficient, \(K_{OW}\), by a constant value:
\[K_{OC} = 0.63 K_{OW}\] (2.9)

The octonal/water partition coefficients for a wide range of compounds are available in the literature (e.g. Leo et al., 1971; Verschueren, 1977; Kenaga and Goring, 1980) and can
FIGURE 2.4  Linear Forms for Graphical Representation of Adsorption Equations
be easily measured in the laboratory. The above formulation (Eq. 2.9) is basically correct if large dispersion coefficients are used to predict breakthrough concentrations, based on field experiments at Ft. Devens, Massachusetts by Tomson et. al., 1985.

With the inclusion of the isotherms, the chemical attenuation factor in the one-dimensional advection-dispersion Eq. 2.1 becomes:

\[
\frac{\rho_b}{n} \frac{\partial c}{\partial t} + \frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} = D \frac{\partial c}{\partial t} - V \frac{\partial c}{\partial x}
\]

(2.10)

Van Genuchten et. al. (1974) used the CSMP computer program to solve Eq. 2.10 with an equilibrium Freundlich Adsorption relationship. The computer model provided a reasonable fit between data and calculated effluent concentration distributed at low seepage velocities through a water saturated loam soil.

Adsorption and dispersion processes have been reviewed in the last two sections. The advection-dispersion equation that includes the adsorption process is a common tool for the prediction of solute transport in the groundwater. Section 2.3 will review the analytical methods currently used to solve the advection-dispersion equation, followed by a discussion of numerical methods in Section 2.4.
2.3 ANALYTICAL METHODS FOR THE TRANSPORT EQUATION

A number of analytical solutions have been derived in the last thirty years for different purposes. Originally, the primary purpose of analytical solutions was to evaluate an aquifer's porosity and dispersion coefficients. More recently, analytical solutions have been used to verify the accuracy of numerical methods. Furthermore, when several parameters for a contaminated field site are insufficiently known, analytical solutions can provide preliminary insight for practical applications.

Most of the analytical solutions assume that the porous medium is homogeneous, isotropic, and saturated. In addition, a steady state ground water flow is generally assumed. Analytical solutions in general were developed for a single recharging well, a slug or continuous contaminant source, and for a recharging-pumping well pair system.

2.3.1 SINGLE RECHARGE WELL SOLUTIONS

Among the single recharge well solutions is the original one-dimensional solution presented by Ogata and Banks (1961). The advection-dispersion equation was reduced to the diffusion equation, similar to the heat conduction equation, by a change of variables. The diffusion equation was then reduced to an ordinary differential equation by application of the Laplace transform, then the Duhamel's theorem, described by Carslaw and Jaeger (1959), was used to obtain the final solution.
Bruch and Street (1967) derived a solution for two-dimensional unsteady dispersion in a one-dimensional steady flow systems via the method of separation of variables. Results are presented in terms of complementary error functions and infinite series. Application of the results requires knowledge of the seepage velocity, the source concentration, and the longitudinal and lateral dispersion coefficients of the prorous medium. Hunt (1978) and Wilson and Miller (1978) obtained similar solutions for the same physical system described by Bruch and Street (1967). In addition, Hunt (1978) presented a three dimensional solution for an instantaneous injection and for a continuous injection at a recarge well. Hunt (1978) used a Taylor series expansion to expand the Hantush well function, the major portion of the two-dimensional solution. Wilson and Miller (1978) claimed that the Laplace's method is a more convenient and accurate technique for the asymptotic expansion of the Hantush well function. Wilson and Miller (1979) demonstrated their solution accuracy through comparisons with the numerical integration of the Hantush well function.

Hoopes and Harleman (1967) presented solutions for a single recharging well in a polar coordinate system. The solutions were developed for continuous injections and for an instantaneous injection of tracer at a steady rate. For the case of a continuous injection at a steady rate, the
solution is not accurate near the source (within 20 particle diameters from the wall) due to an unsatisfied initial condition. An ad hoc approximation, wherein space derivatives were replaced by time derivatives in the dispersive term, was used to obtain the solutions. Hoopes and Harleman's (1967) paper was among the earlier analytical solutions which included the analysis of the effects of both longitudinal and lateral dispersion. Hoopes and Harleman's solutions were used to study the relative influences of dispersion and molecular diffusion on the tracer distribution. Results showed that the dispersion coefficient along the streamlines is the same for both uniform and nonuniform flows at the same velocity.

Gelhar and Collins (1971) presented several solutions with nonuniform flow and variable longitudinal dispersion coefficients. The one-dimensional advection-dispersion equation in curvilinear coordinate systems was reduced to the simple diffusion equation through a series of coordinate transformations. In arriving at this simple diffusion equation, the longitudinal dispersivity was assumed to be small relative to the distance traveled by the front. Solutions were derived for both instantaneous and continuous injection at a recharge well.
2.3.2 Recharge-Pumping Well Pair Solutions

By redefining velocity fields and by matching solutions of the recharge and pumping cycles, the concentration distribution during the pumping cycle of the push-pull test was also obtained by Gelhar and Collins (1971). The nonuniform flow field was implicitly included through integrals, therefore explicit evaluation of the characteristics of the flow field is not required to obtain solutions in their analyses. Dagan (1971) used a perturbation technique to obtain a similar solution to the recharge cycle concentration distribution of Gelhar and Collins (1971). The perturbation solution was built on the stream and potential function domain and was an approximation to the exact solution. The approximated solution approaches the exact solution when the change of the velocity field across the transition zone is small. Eldor and Dagan (1972) extended the perturbation solution for the problem with the addition of radioactive decay and adsorption terms. The general solution is also applied to a recharge-pumping well pair system. However, the solution is inaccurate near the edge of the plume because a relative thick transition zone to the change of the velocity field exists near the edge for a recharge-pumping system.

Hoopes and Harleman (1967) presented a variety of solutions for a recharge-pumping well pair system. These solutions were derived for the following four cases: 1) no
dispersion or diffusion along or transverse to the streamline; 2) dispersion and diffusion along the streamlines but no dispersion or diffusion across the streamlines; 3) dispersion and diffusion transverse to the streamlines, but no dispersion or diffusion along the streamlines; and 4) combined influence of dispersion, diffusion, and advection. Boundary conditions at the recharge well were either a specified constant rate of supply of substance or a constant concentration at the recharge well. The method of Laplace transformations was used to obtain the solution for the case of dispersion along the streamline.

Grove and Beetem (1971) used simple trigonometric equations to describe the length of streamlines and the time for a water particle to flow along any particular streamline from a recharge well to a pumping well. The travel time between two wells represents the solution for the advection equation. By treating each streamtube as a dispersion column of fixed length, Grove and Beetem (1971) combined the dispersion solution by Brenner (1962), the travel time, and the arc length to obtain a complete breakthrough profile of the advection-dispersion equation between two wells (Figure 2.5).

Cleary (1978) used the integral transformation method solved several mass transport equations together with computer programs for these solutions. Cleary's report
contains seven mass transport models and three groundwater flow models. Each of the models has a user-oriented computer program. The mass transport models include one, two, and three-dimensional solutions with different type boundary conditions.

2.4 NUMERICAL MODELING OF GROUNDWATER CONTAMINANT TRANSPORT

Since most analytical techniques treat only ideal homogenous and isotropic porous medium and they are not directly applicable to most field situations, numerical simulation must be considered.

In a nonhomogeneous and anisotropic groundwater flow system, the groundwater seepage velocity is not constant. The character of the advection-dispersion may vary in space and time depending on the velocity field. The advection-dispersion equation becomes a parabolic type partial differential operation if the Peclet number is small. The Peclet number is physically interpreted as a ratio of advective to dispersive transport components. The equation becomes a nearly hyperbolic type partial differential equation if the Peclet number is large, i.e., transport-dominated system. Early numerical experiments for solving the advection-dispersion equation were based on "straightforward" finite differences (Peaceman and Rachford, 1962; Stone and Brian, 1963; Shamir and Harleman, 1967). Finite differences perform well in dispersion-dominated situations
where the Peclet number is small. In a transport-dominated flow system the concentration gradient is usually very steep. Difficulties arise, such as numerical dispersion and oscillations, in the numerical simulation of this sharp front. Many numerical methods have been developed in the last two decades to handle this sharp front. Common numerical approaches for the advection-diffusion equation include the implicit diffusive method, Galerkin finite element and collection methods, alternating direction method, as well as the method of characteristics.

2.4.1 Implicit Diffusive Methods

The implicit diffusive method includes upstream weighted finite difference (Lax and Wendrott, 1964; Chandhari, 1971; Todd et. al., 1972), nine-point finite difference (Yonosik and McCracken, 1979), and Potempa's (1982) method. Upstream weighting is equivalent to adding a numerical dispersion term to the advection-diffusion equation. This method is used because it suppresses nonphysical oscillations, also known as overshoot, in the finite difference solution. Lantz (1971) showed for many practical problems, reducing numerical dispersion sufficiently so as to prevent masking physical dispersion may require an extremely fine grid. One-point upstream weighting finite difference schemes lead to a computational anomaly referred to as the "grid orientation effect". Briefly, the grid orientation effect
refers to a severe dependence of the solution on the spatial orientation of the computational grid. Two-point upstream weighting (Todd, O'dell, and Hiraski, 1972) with a nine-point finite difference scheme (Yanosik and McCracken, 1979) in two dimensions reduces dependence on grid orientation. However, numerical dispersion can still exist. A schematic of the flow directions considered in the five- and nine-point finite difference formulation is presented in Figure 2.6. The five-point formulation only considers flow between a block and the four blocks that are adjacent to its boundaries. The nine-point formulation considers this flow as well as the flow between the block and the four blocks located at its corners.

Potempa (1982) developed an all-balanced finite element procedure which is a hybrid of ideas from block-centered finite difference and piecewise-bilinear finite element methods. For a spatially constant velocity field the finite difference scheme reduces to the nine point scheme of Yanosik and McCracken (1979). Potempa used velocity integrals, rather than pressure differences, to determine flow coefficient, which is the only difference from that of the scheme developed by Yanosik and McCracken.
FIGURE 2.6  Pictorial Representation of the Five- and Nine-Point Finite Difference Formulations (from Yanosik and McCracken, 1979)
2.4.2 Galerkin Finite Element Method

The standard Galerkin finite element method multiplies the advection-dispersion equation by a test function. Then, using Green's theorem and appropriate boundary conditions to obtain a variational form, the accumulation term is usually replaced by a backward finite difference approximation to get an implicit time-stepping scheme. The standard Galerkin finite element method can achieve higher order convergence than the finite difference scheme, and the method is therefore more accurate. The method had been applied to solving the advection-dispersion equation by several authors (Van Genuchten, Pinder, and Frind, 1977; Pinder and Gray, 1977; Gray and Pinder, 1976; Pinder, 1973; Verruijt, 1970; Neuman, Narasimhan, and Witherspoon, 1976; Mercer and Faust, 1981) in the last fifteen years. The strength of finite elements is its ability to handle complex geometry, heterogeneity, and anisotropy. However, the method is much costlier than finite differences, with extra computation in numerical integration and the necessity to solve wider band-width matrices. Further, the nonsymmetric advection term causes difficulties in the linear algebraic system calculation. For advection-dominated flow, the method exhibits oscillations and numerical dispersion.

To reduce oscillations, Huyakorn and Nikuha (1979) employed upstream weighting to finite elements. The upstream finite element scheme is capable of handling steep
concentration fronts. However, it suffers the same numerical dispersion problem as in the upstream finite difference. Collocation methods are even more numerically dispersive because they require a very smooth continuous basis function. The advantage of collocation finite element procedures over Galerkin finite element methods is that the formation of the matrix coefficients is very fast since no integrals need be evaluated or approximated (Percell and Wheeler, 1980).

To avoid high computational cost in the conventional Galerkin finite element formulation, Young (1981) devised a clever way to reduce computing requirements. Young used Lagrange polynomials of degree $r$, $r = 1, 2, \text{ or } 3$, as trial functions and used the Lobatto quadrature rule to integrate the matrix coefficients. The key to the efficiency of this method is that the nodes or grid points in the elements correspond to the evaluation point of the Lobatto quadrature formula. Thus the number of numerical integrations is significantly reduced. For a linear trial function ($r = 1$) and a two-point Lobatto quadrature rule, Young's method reduces to the five-point central difference scheme. Hence, it makes the Galerkin finite element method competitive in costs with the finite difference scheme.
2.4.3 Alternating Direction Methods

To avoid numerical dispersion, another recent trend in the groundwater contaminant transport simulation has been using alternating direction techniques (Peaceman, 1977) with either point collocation (Celia and Pinder, 1982; Wengle, 1982) or finite elements (Frind, 1982; Daus and Frind, 1985). This approach was termed the principal direction technique (PD) (Frind and Pinder, 1982) if formulated in stream function coordinates, and was referred to as an alternating direction Galerkin technique (ADG) if formulated in a coordinate system that is consistent with the principal direction of hydraulic conductivity. The ADG method is more flexible than the principal direction technique in terms of handling anisotropic and heterogeneous groundwater systems. The greatest advantage of this method over the standard Galerkin finite element method is the much reduced computational cost. The computational effort of this method increases only linearly with the grid size while the Galerkin finite element method increases rapidly as the grid size increases. In some cases, the operations count (defined as the total number of multiplications and divisions) of the standard Galerkin method increases with the square of the grid size. The ADG method, because of the explicit direction of the formulation, is restricted by the Courant number, CN, to be less than one to prevent oscillations. Physically, the Courant number relates the
distance a particle travels during one time step to the spatial increment, i.e.:

\[ \frac{V_x \Delta t}{\Delta x} \]

The mesh Peclet number also is restricted to be less than two as reported in Daus and Frind (1985). The major drawback of the ADG method is the grid orientation problem, and the ADG method may not be able to handle random hydraulic conductivity effectively.

2.4.4 Method of Characteristics

In order to avoid numerical dispersion and oscillation in numerical simulation of the advection-dispersion equation, a moving point method was suggested by Garder et. al. (1964). In this approach, advection is handled by the method of characteristics applied to a set of moving particles. The dispersion part of the problem is solved by an explicit finite difference scheme on a fixed grid. The solution values are interpolated to the fixed grid from the moving points which treat the advection part of the problem. Dispersion is estimated on the fixed grid and interpolated to the moving point.

The computer model of the two-dimensional solute transport and dispersion model in groundwater, developed by Konikow and Bredehoeft (1978) of the U. S. Geological Survey (USGS) was based on this method. The model uses fixed
block-centered finite difference grids on a rectangle and places a number of particles in each grid cell. For each time step, every particle is moved a specified distance along a characteristic curve. At the end of the time step, the concentration at each node is temporarily assigned the average of the concentrations of all particles that are located within the grid cell, which accounts for the advective part of the equation. The changes in concentration caused by hydrodynamic dispersion, fluid sources, divergence of velocity, and changes in saturated thickness are calculated using an explicit finite-difference approximation. This change in concentration is then added to the concentration change produced by the advective particles. Figure 2.7 illustrates the moving particle concept. The USGS model is one of the most widely used groundwater transport models due to several of its flexible features: arbitrary placement of injection and withdrawal wells, spatially varying diffuse recharge or discharge, and time-variable pumping periods.

The major drawback of the moving point method arises in the interpolation from the moving points to the fixed grid at high Peclet number. Numerical experiments by Price, Cavendish, and Varga (1968) demonstrated the method does not converge under mesh refinement as the mesh Peclet number goes to zero. The conventional method of characteristics has the problem of maintaining a material balance and
FIGURE 2.7 Moving Particle Concept
also the practical limitation of the time-step size. Farmer (1985) showed that many moving point algorithms are inconsistent and accordingly modifications were described so that convergence can be obtained. Using the moving point idea, Farmer (1985) developed a hybrid moving point method. The method interpolates between a moving point and a fixed mesh Peclet number. At low Peclet numbers the method uses the fixed mesh algorithm and at high peclet numbers a modified moving point algorithm is used. This is analogous to local adaptive mesh refinement in the context of fixed mesh algorithms. Numerical experiment by Farmer (1985) showed that the hybrid moving point method converges under fixed-mesh refinement but not under an increase in the number of moving points per cell.

Recent work by Ewing, Russell, and Wheeler (1983) has produced a very efficient and accurate modified method of characteristics (MMOC) for modeling incompressible miscible displacement in porous media. The MMOC uses characteristics to model advection and finite element for diffusion and dispersion. The crucial aspect of this method both theoretically and computationally is the approximation of the time derivative. Many methods based on characteristics fix a point at the current time level and ask where it will go at the advanced time level. These moving point or front tracking methods must then solve at the advanced time on a grid of irregular or unpredictable character. The MMOC
takes the opposite view, fixing a point at the advanced time level and asking where it came from at the current time level. Thus, the solution grid at the advanced time level is controlled by the method, not the flow. The one-dimensional flow follows a characteristic path that translates concentration profiles at two time steps is shown in Figure 2.8. It has been shown that the MMOC eliminated numerical dispersion and grid orientation, and greatly reduced numerical oscillation problems. In this method much larger time steps can be used with no loss of accuracy.

Results of numerical experiment by Russell (1982) showed that the MMOC method takes twenty-five times larger time steps than the standard Galerkin method to achieve the same size of spatial error in a one-dimensional simulation. However, the MMOC method is not totally without problems. The MMOC method is formulated in nondivergence form, and it has some material balance error. When higher injection rates are introduced, the material balance error becomes obvious. It may reach three per cent material balance error under steep concentration gradient and relatively coarse grid system.

The modified method of characteristics has also been developed independently by Neuman (1981, 1982) who reported success in coupling the MMOC with a moving particle method in the neighborhood of fronts. When steep advective concentration fronts are present, Neuman used an empirical
\[ \frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} - D \frac{\partial^2 c}{\partial x^2} = 0 \quad x \in [0, 1] \]

\[
\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = \frac{c^{*+}'(x) - c^n(x-v\Delta t)}{\Delta t}
\]

**FIGURE 2.8** Schematic One-Dimensional Representation of the MMOC Model
formula to track forward with the aid of moving particles. Away from the steep front, the advective front is handled by the modified method of characteristics similar to the procedure by Russell (1982). The major difference between Neuman and Russell's approach is the way grid space is handled. Russell used a fixed space-time grid for both the advective part and the dispersal part of the equation, while Neuman used two different space-time grids for these two parts and projected results from one grid to another, which led to some numerical dispersion as reported by Neuman (1982).

2.5 FIELD SITE APPLICATIONS

The ultimate objective of analytical solutions and numerical modeling is to provide tools to understand the behavior of subsurface contaminant movement and to extrapolate future conditions based on past and present activities. In addition to mathematical modeling in pursuit of this objective, it is also necessary to understand the behavior of the full scale contaminant transport at field sites. Field studies combined with mathematical modeling are useful in evaluating the role of various transport mechanisms, in evaluating the accuracy of mathematical models, and in providing confidence in sensitivity analyses for various remedial measures. Detailed field studies include geophysical surface and borehole mapping, land
surveys, hydrogeochemical measurements, chemical composition evaluations, hydrogeological descriptions, and large-scale dispersion and adsorption studies.

2.5.1 Groundwater Parameters

Several parameters must be determined prior to evaluating groundwater contaminant transport. These parameters may broadly be grouped under three categories; groundwater hydraulics, transport mechanisms, and boundary conditions. Groundwater hydraulic parameters include hydraulic conductivity, aquifer thickness, potentiometric map of the water table, leakage rates, specific yield, recharge rate, storage coefficient and porosity. Transport mechanisms include diffusion, dispersion, adsorption equilibrium, and sources of contamination such as ponds or wells. Boundary conditions can either be specified as no flow boundaries or as constant head boundaries. No flow boundary refers to an impermeable aquifer, e.g. clay or synthetic membrane. Constant head boundary is usually applied for known water table elevations or known piezometer heads.

The first and the most important parameter for a contaminated site investigation is the hydraulic conductivity. Values of hydraulic conductivity for an aquifer can be obtained from grain-size analyses, from water level response tests in piezometers, from pumping tests, and
from permeameter tests on two disturbed core samples (MacFarlane et al. 1983; Freeze and Cherry, 1979; Todd, 1980; Davis and De Wiest, 1966). Pumping tests also provide in situ measurements of the aquifer thickness and the storativity based on various forms of Theis solutions. The measured conductivity, aquifer thickness, and storativity are used to calculate the groundwater seepage velocity and to determine the travel paths that contaminants will follow. One usually uses numerical models or analytical solutions as aids to delineate the flow field from which subsequent analyses on various remedial schemes can be evaluated.

The porosity \( n \) can be an important controlling influence on hydraulic conductivity \( k \) and is a necessary parameter for determining the Darcy velocity. Porosity can be calculated by a simple arithmetic equation (Freeze and Cherry, 1979).

\[
n = 1 - \frac{\rho_b}{\rho_s}
\]

where \( \rho_b \) is the bulk mass density of the sample and \( \rho_s \) is the particle mass density. In general, porosity is in the range of 0.25 - 0.5 for unconsolidated deposits. Porosity can also be determined by a field technique using an analytical solution developed by Grove and Betem (1971).

While it is possible to calculate the rate of recharge or leakage based on either the Darcy's law or a hydrologic budget, the response of the water table under various climate conditions for different geologic environments are
very complex. Therefore, the rate of recharge or leakage in many case studies become fitted parameters by trial-and-error procedures from numerical simulations.

2.5.2 Field Applications Using Models

Increasing awareness of the problems presented by industrial chemical dumps and landfill operations is leading toward an increased interest in, and application of computer models. This section will present several representative field sites where computer models have been applied. One of the earliest and more extensively studied field sites in the United States is located at Long Island, New York. A metal-plating-waste effluent containing cadmium and hexavalent chromium from an industrial plant was discharged to disposal basins and subsequently seeped down into the upper glacial aquifer. An extensive field site investigation was first conducted by Perlmutter and Lieber (1970). They characterized the hydrologic system which included the infiltration rate, water bearing capacity of the aquifer, and the rate of plume movement. Pinder (1973) continued the field study using a two-dimensional finite element model developed for the mass transport equation. Much more detailed understanding of the hydrological system and ultimate fate of the contaminated plume were illuminated by the numerical simulation. Wilson and Miller (1978) used an analytical solution and predicted the observed plume by Perlmutter and Lieber.
Anderson et. al. (1984) used a finite difference model for groundwater flow, developed by Trescott et. al. (1976), to help interpret groundwater flow and convective transport at the Lipari landfill, New Jersey. Analytical solutions were used to provide an extra check on the results of the numerical models. The finite difference model was also used to design a slurry wall, drain location, drain depth, and a clay cap at the Lipari landfill site. As an alternative remedial scheme, using fresh water to flush the contaminated site was assessed quantitatively by an analytical Theis solution. Flushing by wells at the Lipari site was found infeasible due to the small head differential between injection and pumping wells.

Gray and Hoffman (1983) developed a steady state two-dimensional finite element flow model and used the model to study Price's landfill site in New Jersey. Toxic chemicals including acetone, acid, chloroform, hexane, xylene, ethylene dichloride, and toluene were found at Price's landfill site. History of conditions of contamination and water-quality data were unavailable, therefore sensitivity analyses which included a variety of parameter variations were simulated. Pump tests were conducted to estimate the transmissivity using Thiem's analysis. An injection-pumping remedial scheme was selected and tested by the computer model.
By far the most thoroughly reported and studied field site in the world is the Borden landfill site in Canada (Figure 2.9). The Borden landfill site is located within the confines of the Canadian Force Base, 80 km northwest of Toronto, Ontario (MacFarlane et. al., 1983). Landfilling operation at the Borden site spanned a period of 36 years, from 1940 to 1976. Field site investigations, conducted by Gartner Lee Associates Ltd. and the University of Waterloo, began in 1974 when Gartner Lee Associate Ltd. installed 51 piezometers and water-table standpipes at 26 locations. Spatial distribution of the contaminated zone was delineated in detail by measurements of electrical conductance on groundwater samples obtained using auger-head samples designed specifically for the task (Anderson, 1977; Cherry et. al., 1983).

Sudicky et. al. (1983) performed a natural gradient test at the Borden landfill to determine dispersivity values in three principal direction at the site. A three-dimensional analytical solution, described by Carslaw and Jaeger 1959, to the advection-dispersion equation was used to fit the field data. They discovered that in order to obtain matches with the observed concentration at larger values of migration distance, the dispersivity had to be steadily increased. An estimate of minimum average recharge through the landfill that had occurred since 1953, was calculated using tritium as an indicator (Egboda et. al., 1983).
FIGURE 2.10 Conroe Hazardous Waste Site
The hydrogeochemical effects on the contaminant transport at the site was studied by Nicholson et. al. (1983) and Dance and Reardon (1983). They concluded that in permeable geologic deposits, contaminants not affected by chemical attenuation can be transported over great distance.

There are only a few other modeled case studies reported in the literature. An abandoned creosote waste facility in Conroe, Texas had been studied for two years as a research site for the National Center for Groundwater Research at Rice University by Bedient et. al. (1984) (Figure 2.10). The hydrology of the site and surrounding areas was clay and sand lenses of a meander belt overlying a delta sand with 25 to 30 ft depth to the water table. The site was characterized by sampling soils and water quality at 14 monitoring wells and 35 boreholes. Contaminant migration was measured and compared to prediction from the USGS solute transport model (Konikow and Bredehoeft, 1978). Based on the model projections for the conservative chloride plume, the retardation of adsorbing organics was estimated. Freeberg (1985) used the USGS solute transport model to evaluate remedial schemes at an industrial waste site contaminated by trichloroethylene and other industrial solvents.

This review only illustrates several representative field studies. Although deeper understandings are gained by reviewing many field site studies, to date one still has to
go through all the sampling procedures for a particular field site investigation in order to define the groundwater system, the pollutant-transport mechanisms, the nature and rates of chemical, physical, and biological transport and hopefully be able to develop an efficient remedial scheme for the site. These sampling procedures are not only time-consuming but are also very expensive. A thorough compilation and synthesis for field study encompassing every possible groundwater system and geological informations would be a helpful guide for future site-specific study.
CHAPTER THREE

NUMERICAL METHODS FOR SOLUTE TRANSPORT AND GROUNDWATER FLOW

Numerical simulation of groundwater contaminant transport involves solving a solute transport equation and a groundwater flow equation for a two-component single phase system. These two equations are solved sequentially or simultaneously if the groundwater flow is transient, and they are solved independently if the groundwater flow is in steady state. Mathematically, the solute transport processes are described by an advective-dominated parabolic partial differential equation. The partial differential equation incorporates the significant physical and chemical processes such as advection, hydrodynamic dispersion, mixing from fluid sources, and reactions, which govern the transport in the groundwater regime. Having discussed and reviewed the physical and chemical phenomena in Chapter Two, the following section introduces the partial differential equations that describe groundwater contaminant transport processes.

3.1 MATHEMATICAL FORMULATION OF SOLUTE TRANSPORT PROCESSES

The general solute transport equation is a statement of the balance of the time rate of increase of total mass at a point, the divergence of the mass flux vector, and the source strength which includes injection wells, diffuse recharge, and reactions.
The general three-dimensional solute transport equation has been derived as follows:

$$\frac{\partial m}{\partial t} + \nabla \cdot (b \overline{J}) = Nc' + Qc'' + G$$  \hspace{1cm} (3.1)

where $m =$ the solute mass per bulk volume (solution and sorbed phase)
$t =$ time
$\overline{J} =$ total mass flux
$N =$ diffuse recharge or leakage
$c' =$ concentration of diffuse recharge or leakage
$c'' =$ concentration of injection well recharge
$Q =$ point source and sinks (Dirac measures)
$G =$ source strength from reactions
$b =$ aquifer thickness

The total mass flux includes transport by advection and hydrodynamic dispersion:

$$\overline{J} = \nabla c - D \cdot \nabla c$$  \hspace{1cm} (3.2)

where $c =$ solute concentration
$D =$ hydrodynamic dispersion tensor

$$D = n D_m I + \frac{\alpha_L}{|V|} \begin{vmatrix}  \nabla x^2 & \nabla x \nabla y \\ \nabla x \nabla y & \nabla y^2 \end{vmatrix} + \frac{\alpha_T}{|V|} \begin{vmatrix} \nabla y^2 & -\nabla x \nabla y \\ -\nabla x \nabla y & \nabla x^2 \end{vmatrix}$$

where $n =$ porosity
$\alpha_L =$ longitudinal dispersivity
$\alpha_T =$ transverse dispersivity
$D_m =$ effective diffusion coefficient
$I =$ unit tensor
$\nabla x, \nabla y =$ components of Darcy velocity
This dispersion tensor was derived by Peaceman (1966). If one expands the divergence in Eq. 3.1 by assuming that the aquifer thickness is constant and makes use of Eq. 3.1, one obtains

$$b \frac{\partial m}{\partial t} + b \nabla \cdot (\bar{V}c - \bar{D}c) = Nc' + Qc'' + G \quad (3.3)$$

Now consider the nature of the sorption and reaction terms. The total mass $m$ includes both the solute mass and the sorbed mass. If $c$ is the sorbed mass concentration in mass per mass of soil, and $\rho$ is the bulk density of the soil, then

$$m = nc + \rho \bar{c}$$

The sorbed and solute concentration are related through a general sorption isotherm of the form

$$\bar{c} = F(c)$$

If the sorption is sufficiently rapid so that equilibrium applies then

$$\frac{\partial m}{\partial t} = \frac{n + \rho F'}{\partial t} - \frac{\partial c}{\partial t} \quad (3.4)$$

where $F'$ is the slope of the sorption isotherm at concentration $c$. If $F'$ is a constant (called the partition coefficient), then the resulting isotherm is linear. Otherwise, the term is nonlinear. Finally, the reaction term $G$, which is inherently a kinetic term, may be of any order. This research considers only linear isotherms and
does not include either the reaction or the leakage term for the simplicity of analyses. Nonlinear isotherms have not been proven to be practical in the field applications due to lack of measurements. Most groundwater systems are expected to exist in the linear first order portion for most processes of interest (Bedient et. al., 1981). The final form of the mass transport equation is:

\[
\frac{\partial c}{\partial t} + b(n + \rho F') - b\mathbf{v} \cdot (\nabla c - \nabla \mathbf{v} c) = Q c''
\]  

(3.4)

If both sides of Eq. 3.4 are divided by the thickness of the aquifer, b, Eq. 3.4 becomes

\[
\frac{\partial c}{\partial t} + nR_d\frac{\partial c}{\partial t} + \mathbf{v} \cdot (\nabla c - \nabla \mathbf{v} c) = q c''
\]  

(3.5)

where \(R_d = 1 + \rho/n(F')\), the retardation factor

\(q = Q/b\) , injection rate per unit thickness

Eq. 3.5 is the governing differential equation solved by the modified method of characteristics. Typical one-dimensional solutions as functions of time and distance are shown in Figure 3.1.

3.2 MODIFIED METHOD OF CHARACTERISTICS

Eq. 3.5 is a parabolic-type partial differential equation; if the hydrodynamic dispersion, D, were zero, Eq. 3.5 would be a hyperbolic equation. It is well known that solutions for hyperbolic-type equations can be represented
FIGURE 3.1 Typical One-Dimensional Concentration Profiles as Functions of Time and Distance
from the initial data propagating over well-defined paths in the surface. These propagation paths are called characteristics. Motivated by the hyperbolic case, the solution for the advective-dominated advection dispersion equation is defined by characteristic curves in the direction of flow. The characteristic solutions can be viewed as small dispersion away from these characteristic curves, along which concentration, \( c \), is a smooth function (Ewing and Russell, 1981). The overall idea is to let the concentration of a fluid particle move along the characteristics of the hyperbolic problem obtained by ignoring dispersion. This treats the advection part of the problem, which is the difficult part numerically; then finite-elements are used for the dispersion part, for which they are well suited.

Consider a rectangular domain, \( \Omega \), with the same concentration on both sides of the boundary, i.e., the concentration flux crossing the boundary in the direction of a unit outward normal, \( \eta \), to the boundary \( \partial \Omega \) is zero;

\[
\nabla c \cdot \eta = 0 \quad x \in \partial \Omega, \quad 0 \leq t \leq T
\]

and an initial condition

\[
c(x,0) = 0 \quad x \in \Omega
\]

To apply the modified method of characteristic procedure, the advection term needs to be separated out so that it can stand alone. Using the product rule on the \( \nabla \cdot (\nabla c) \) term, move the \( (\nabla \cdot \nabla) c \) term to the right hand side of Eq. 3.5 to obtain:
\[
\frac{\partial c}{\partial t} + \nabla \cdot (\bar{V} c) + \nabla \cdot V c = (c^n - c)q \tag{3.7}
\]

Define the unit vector, \( \tau(x,t) \), in the characteristic direction such that

\[
\frac{\partial}{\partial \tau(x,t)} = \frac{nR_d}{\sqrt{\bar{V}^2 + (nR_d)^2}} \frac{\partial}{\partial t} + \frac{\bar{V} \cdot V}{\sqrt{\bar{V}^2 + (nR_d)^2}}
\tag{3.8}
\]

Eq. 3.7 can be rewritten as

\[
\sqrt{\bar{V}^2 + (nR_d)^2} \frac{\partial c(x,t)}{\partial \tau} - \nabla \cdot (\bar{V} c) = (c^n - c)q \tag{3.9}
\]

Eq. 3.9 is the non-divergence form of the transport equation. Notice here \( c \) no longer represents concentration at a fixed point in space time, rather the concentration along the characteristics that follow the flow.

Approximating the characteristic derivative by a backward finite difference procedure, one obtains:

\[
[\bar{V}^2 + (nR_d)^2]^{1/2} \frac{\partial c}{\partial \tau}(x,t)
= [\bar{V}^2 + (nR_d)^2]^{1/2} \frac{c(x,t^{n+1}) - c(\bar{x},t^n)}{[(x-\bar{x}) + (\Delta t)^2]^{1/2}}
= nR_d \frac{c(x,t^{n+1}) - c(\bar{x},t^n)}{\Delta t} \tag{3.10}
\]

where \( \bar{x} = x - \frac{\bar{V}^*}{nR_d} \Delta t \tag{3.11} \)

In Eq. 3.11, \( \bar{V}^* \) is an approximated average velocity of a fluid particle reaching \( x \) at time \( t^{n+1} \), the values of \( \bar{V}^* \) are extrapolated from the last two time steps using a Taylor series expansion:
\[
\bar{V}^*(x, t^{n+1}) = \bar{V}(x, t^n) + \bar{V}'(x, t^n)(t^{n+1} - t^n) + \cdots \\
= \bar{V}(x, t^n) + \frac{\bar{V}(x, t^n) - \bar{V}(x, t^{n+1})}{(t^{n+1} - t^n)}(t^{n+1} - t^n) \quad (3.12)
\]

If the time steps are uniform Eq. 3.12 becomes:

\[
\bar{V}^*(x, t^{n+1}) = 2\bar{V}(x, t^n) - \bar{V}(x, t^{n-1}) \quad (3.13)
\]

Substituting Eq. 3.10 into Eq. 3.9 one obtains:

\[
\frac{c(x, t^{n+1}) - c(x, t^n)}{\Delta t} - \bar{V}^*(x, \bar{V}^*)\frac{\partial c}{\partial \bar{V}}c^{n+1} = (c^* - c)_q^{n+1} \quad (3.14)
\]

Clearly, in order to evaluate the difference quotient appeared in the first term of the left hand side of Eq. 3.14, one must be able to determine \( \bar{x} \) and \( \bar{V}^* \) accurately.

The following section will describe the micro-time steps from which vectors of \( \bar{x} \) and \( \bar{V}^* \) are obtained.

### 3.2.1 Segmenting Description

The velocity varies rapidly in space near wells, therefore it requires to use small micro-time steps to trace along the characteristics (see Figure 3.2). In Figure 3.2, the one-time step \( \Delta t \) is divided into several micro-time steps \( \Delta t_i \), \( i = 1, 2, \ldots, m \), starting at a fixed Gauss point, \( x \), at time level \( t^{n+1} = t_0 \) to trace back through the tangent of characteristics, until the time step \( \Delta t \) is exhausted.

The crucial aspect of the modified method of characteristics, both theoretically and computationally, is
FIGURE 3.2 Micro-time Step
the tracing backward in time instead of forward in time as in front tracking methods of characteristics. By fixing a point at the advanced time level and asking where it came from at the present time level, the need for changing grid space at every time step is eliminated. A fixed grid space can be used for all time.

To compute \( \mathbf{v}^* \) accurately near wells, a predictor-corrector procedure is involved. At the start of each iteration of micro-time step, say \( t_k \) and

\[
t_k = t_0 - \sum_{m=1}^{k} (\Delta t_m)
\]

where \( t_0 \) is the advanced time and \( t_k \) is the time associated with \( x_k \) on the space-time characteristic, evaluating the velocity \( \mathbf{v}_k \) at time \( t_k \) and space \( x_k \) by a bilinear interpolation on the velocity field. After \( \mathbf{v}_k \) is evaluated, moving backward a distance from \( x_k \) dictated by the velocity \( \mathbf{v}_k \) i.e.,

\[
x_{k+1} = x_k - \frac{\mathbf{v}_k}{nR_d} \Delta t_k
\]

This is a predictor for the next segment of the characteristic. To get a corrector, evaluate the velocity \( \mathbf{v}_k \) which is associated with time \( t_{k+1} \) and space \( x_{k+1} \). The final velocity of the segment will be the average of \( \mathbf{v}_k \) and \( \mathbf{v}_k \) i.e.,

\[
\mathbf{v}_k = 0.5(\mathbf{v}_k + \mathbf{v}_k)
\]
Then use the averaged velocity, $\bar{V}_k$, to calculate the corrected segment, namely

$$x_{k+1} = x_k - \frac{\bar{V}_k}{nR_d} \Delta t$$

Then repeat the predictor-corrector procedure until the time step $\Delta t$ is exhausted and a point $\bar{x}$ is determined. The final velocity, $\bar{V}^*$, which takes the characteristic from the initial point $x$ to the final point $\bar{x}$ is then equal

$$\bar{V}^* = (x - \bar{x})nR_d/\Delta t$$

Notice the time-stepping procedure defined by Eq. 3.14 will require the evaluation of $c$ at $\bar{x}$ at time level $t^n$. Since this point, in general, does not lie at a grid point, some type of interpolation is necessary to evaluate it. The finite element case requires no interpolation since the elements already do it. If $\bar{x}$ reaches across the boundary $\partial \Omega$, use the no-flow boundary condition as a reflection to bring it back.

It remains to show how $\Delta t_k$ is chosen. This is done via a crude error estimator that assumes that the velocity field behaves like the inverse of the distance, $1/r$, to the nearest well from a Gauss quadrature point. The error of the predictor-corrector velocity from the exact averaged velocity will be about $1\%$, if the predictor-corrector velocity moves $2/3$ of the distance from a Gauss point to a pumping well or $1/3$ of the distance from an injection well
(within the time limit $\Delta t_k$). The following section will briefly introduce the mathematical derivation of the micro-time step $\Delta t_k$.

3.2.2 Micro-time Step

Suppose a quadrature point is at a distance $r_0$ to a pumping well, the velocity $V(r_0)$ is then equal to $c/r_0$ and it will move to a distance $(1 + \varepsilon)r_0$, in time segment $\Delta t$, i.e.,

$$\frac{c \Delta t}{r_0 nR_d} = \varepsilon r_0$$

Corrected velocity is then equal to

$$0.5[1 + 1/(1+\varepsilon)]V(r_0)$$

which moves to an approximated distance

$$\left[ \frac{\varepsilon}{1 + (1 + \frac{1}{2\varepsilon})} \right] r_0$$

The exact distance is determined by solving an ordinary differential equation

$$r'(t) = \frac{V(r(t))}{nR_d}$$

$$\rightarrow r(t)r'(t) = \frac{c}{nR_d}$$

$$\rightarrow (r^2(t))' = \frac{2c}{nR_d} \tag{3.15}$$

Given the initial condition $r(0) = r_0$, Eq. 3.15 has the solution
\[ r^2(\Delta t_k) = r_o^2 + \Delta t_k \cdot \frac{2c}{nR_d} \]
\[ = r_o^2 + 2\varepsilon r_o^2 \]
\[ = r_o^2(1 + 2\varepsilon) \]

Therefore the exact move is \( \sqrt{(1 + 2\varepsilon)} r_o \).

Define error = (approximated move - exact move)/exact move
\[
\frac{\varepsilon}{2} \left( 1 + \frac{1}{1 + \varepsilon} \right) - (\sqrt{1 + 2\varepsilon} - 1) \]
\[ = \frac{\sqrt{1 + 2\varepsilon} - 1}{\sqrt{1 + 2\varepsilon} - 1} \]

Suppose \( \varepsilon = 2/3 \), then the approximated move = 0.5333, the exact move = 0.5275, and the error = (0.5333 - 0.5275) = 1.1%.

The above derivation is from a quadrature point at a pumping well, a similar error estimator from an injection well to a quadrature point can follow the same procedure.

3.2.3 Finite Element Methods

A Standard Galerkin finite element method is used for the spatial discretization. Briefly, the method involves dividing the domain of the solution into a finite number of simple subdomains, the finite element, and using variational concepts to construct an approximation of the solution over the collection of finite elements.

The variational statement of the problem is set up as follows. Multiply Eq. 3.14 by a sufficiently smooth test
function \( V \), integrate over the spatial domain \( \Omega \), and integrate by parts which yields,

\[
\iiint_\Omega \left( \frac{c(x,t^n) - c(x,t^{n+1})}{\Delta} V + D(x,V^*)V c^{n+1} \cdot V - V \cdot [V D(x,V^*)V c] \right) \, dx \, dy \\
= \iiint_\Omega \left( c^n - c^{n+1} q^{n+1} V \right) \, dx \, dy
\]  
(3.16)

The last term in the left hand side of Eq. 3.16 can be transformed into boundary integrals using the divergence theorem:

\[
-\iiint_{\partial \Omega} V \cdot (V D(s,V^*)V c) \, dx \, dy \\
= -\iiint_{\partial \Omega} \frac{\partial c}{\partial \eta} \, ds \\
= -\iiint_{\partial \Omega} \frac{\partial c}{\partial \eta} \, ds \\
= -\iiint_{\partial \Omega} \left( D_{xx} \frac{\partial c}{\partial x} + D_{xy} \left( \frac{\partial c}{\partial y} \frac{\partial x}{\partial y} + \frac{\partial c}{\partial x} \frac{\partial y}{\partial y} \right) + D_{yy} \frac{\partial c}{\partial y} \frac{\partial x}{\partial y} \right) V \, d\sigma
\]
(3.17)

The \( D_{xx} \) and \( D_{yy} \) terms are zero because of Eq. 3.6, and the \( D_{xy} \) terms contain the product \( V_x V_y \), which is zero on all boundary edges if the no flow boundary condition is also applied to the groundwater flow equation. A more detailed discussion on the boundary conditions will be presented in a later section.

If the boundary terms all vanish, after some rearrangements, Eq. 3.16 becomes:
\[
\int_{\Omega} (nRdC^{n+1}v + v\Delta tD_{xx}(x, \bar{v}^a)) \frac{\partial c^{n+1}}{\partial x} \frac{\partial v}{\partial x} dx dy \\
+ \Delta x D_{xy} \left( \frac{\partial c^{n+1}}{\partial x} \frac{\partial v}{\partial y} + \frac{\partial c^{n+1}}{\partial y} \frac{\partial v}{\partial x} \right) dx dy \\
+ \Delta t \sum_{i=1}^{n+1} c_i q_i^{n+1} V(W_i)
\]

\[= \int_{\Omega} nRdC^n(x)v(x) dx dy + \Delta t \sum_{i=1}^{n+1} q_i^{n+1} V(W_i) \quad (3.18)\]

The source term \(q^{n+1}\) now appears with non-zero coefficient only at injection wells, \(W_i\), where it takes the form \(q_i^{n+1} \delta_i\) for \(q_i^{n+1} > 0\).

Eq. 3.18 completes the procedure which combines the modified method of characteristics with Galerkin finite element methods, for the simulation of the transport equation. Note that the advection term, \(C^n(x)\), is moved to the right hand side of Eq. 3.19, so that the system of linear equations is symmetric and positive-definite. This makes the method ideal for iterative linear-solution algorithms, such as preconditioned conjugate gradient method, in large problems.

Douglas and Russell (1982) analyzed this procedure theoretically. The usually \(||\partial^2 c/\partial t^2||\Delta t\) temporal error estimate was replaced by \(||\partial^2 c/\partial t||/\Delta t\) which should be much smaller because the true solution changes much less rapidly
along characteristics that follow the flow than it does at a fixed point in space. Thus, there is a reason to expect much larger time steps to be feasible and accurate with this method than with standard Galerkin finite element method.

3.2.4 Spatial Discretization

It is mentioned in section 3.2.3 that the test function is a sufficiently smooth function. More elaborative descriptions of test and trial spaces are given in this section.

To construct the space of trial functions and test functions, some notations have to be introduced first. Let \( \Omega = \{a_x, b_x\} \times \{a_y, b_y\} \)
and divide \( \Omega \) into \( N_x \times N_y \) blocks.
Let \( \Delta x = \{a_x = x_0 < x_1 < \cdots < x_{N_x} = b_x\} \),
\( \Delta y = \{a_y = y_0 < y_1 < \cdots < y_{N_y} = b_y\} \),
as subdivisions in \( x \) and \( y \), respectively. Define the space \( M_k(r, \Delta x) \) to be the set of all piecewise polynomials of degree \( r \) defined on the grid \( \Delta x \) and have \( k \) continuous derivatives on the interval of interest. For notation purposes, define the space
\[
M_k(r, \Delta x) = \{ \psi \in c^k([a_x, b_x]) : \psi|[x_{i-1}, x_i] \in P_r \text{ for } i = 1, 2, \ldots, N_x \}
\]
\( P_r \) is the set of all polynomials of degree \( r \) defined on \( [x_{i-1}, x_i] \), and if \( \psi \in c^k \), then \( \partial^m \psi / \partial x^n \) are continuous on \( [a_x, b_x] \) for all \( n \leq k \).
After defining notations, the space for test functions and trial functions for the transport equation can be introduced as follows.

The space is a tensor product space $M_0(l,\Delta x) \times M_0(l,\Delta y)$ which refers to continuous piecewise bilinears on the square. A continuous piecewise bilinear function consists of all linear combinations of the form

$$c(x,y) = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} \beta_{ij} V_i(x) W_j(y), \quad 0 \leq i < N_x, \quad 0 \leq j < N_y$$

where $V_i(x)$ and $W_j(y)$ denote the one-dimensional piecewise linear basis functions in each direction which are equal to one at the indexed node and zero at all other nodes, i.e.,

$$V_i(x) = \begin{cases} \frac{x - x_{i-1}}{h_i} & \text{for } x_{i-1} \leq x \leq x_i \\ \frac{x_{i-1} - x}{h_{i+1}} & \text{for } x_i \leq x \leq x_{i+1} \\ 0 & \text{for } x < x_{i-1} \text{ and } x > x_{i+1} \end{cases}$$

where $h_i = x_i - x_{i-1}$, is the length of an element in the $x$ direction and

$$W_j(y) = \begin{cases} \frac{y - y_{j-1}}{h_j} & \text{for } y_{j-1} \leq y \leq y_j \\ \frac{y_{j-1} - y}{h_{j+1}} & \text{for } y_j \leq y \leq y_{j+1} \\ 0 & \text{for } y < y_{j-1} \text{ and } y > y_{j+1} \end{cases}$$
3.2.5 **Lobatto Quadrature Rule for the Integrals**

The Lobatto quadrature integration formula was first applied in finite element methods by Young (1981). The key to the efficiency of this formulation is that the nodes or grid points in the elements correspond to the evaluation points of the Lobatto quadrature formula. The computational work of numerical integration is cut significantly. The popular Simpson's integration rule is a three-point Lobatto quadrature rule, which integrates continuous piecewise bilinears exactly. Other than significant reductions of computational work, the Lobatto quadrature rule is particularly useful for the modified method of characteristics. The characteristics defining $x$ crosses element boundaries and does not conform to the grid, it is required to use a rule that includes integration points on element boundaries so that informations from adjacent elements can be linked together, therefore the most natural choice is the Lobatto quadrature rule.

3.2.6 **CONCENTRATION DISTRIBUTION AT EARLY TIME USING RADIAL FLOW**

Early in the injection the influence of other pumping wells are negligible in the neighborhood of the injection well. Thus, for a certain period the concentration is essentially radially symmetric about the well. However, unless a very fine mesh is used, radially symmetric
functions and sharp fronts at early times are not well represented by the tensor product piecewise bilinear functions. It is feasible to reduce the concentration to a one-dimensional radial model independent of hydraulic heads. This is an idea of Douglas et. al. (1983).

The general non-divergence form of the advection-dispersion equation is:

\[
\frac{\partial c}{\partial t} nR_0 + V \cdot \nabla c - V \cdot (D \nabla c) = 0, \quad 0 \leq r \leq R, \quad 0 \leq t \leq t_f \tag{3.19}
\]

\[
\frac{\partial c}{\partial t} (0, t) - \alpha \frac{\partial c}{\partial r}(0, t) = c, \quad 0 \leq t \leq t_f
\]

\[
c(R, t) = 0, \quad 0 \leq t \leq t_f
\]

\[
c(r, 0) = 0, \quad 0 \leq r \leq R
\]

Here \( c = c(r, t) \) represents concentration at a radial distance \( r \) from the well. Eq. 3.19 can be transformed to a polar coordinate system by the change of variables:

\[
x = r \cos \theta \]

\[
y = r \sin \theta
\]

and

\[
\frac{\partial c}{\partial r} = \frac{\partial c}{\partial s} \cos \theta + \frac{\partial c}{\partial y} \sin \theta
\]

\[
\frac{\partial c}{\partial \theta} = -\frac{\partial c}{\partial x} \sin \theta + \frac{\partial c}{\partial y} \cos \theta
\]

\[
\frac{\partial^2 c}{\partial r^2} = \frac{\partial^2 c}{\partial x^2} \sec^2 \theta + \frac{\partial^2 c}{\partial x \partial y} \sin \theta \cos \theta + \frac{\partial^2 c}{\partial y^2} \sin^2 \theta
\]
\[ \frac{\partial^2 c}{\partial \theta^2} = \frac{r^2 \sin^2 \theta}{\partial x^2} - 2r^2 \sin \theta \cos \theta \frac{\partial^2 c}{\partial x \partial y} \\
+ r^2 \cos^2 \theta \frac{\partial^2 c}{\partial y^2} - r \cos \theta \frac{\partial c}{\partial x} - r \sin \theta \frac{\partial c}{\partial y} \]

Thus,

\[ \nabla^2 c = \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \]

\[ = \frac{\partial^2 c}{\partial x^2} (\cos^2 \theta + \sin^2 \theta) + \frac{\partial^2 c}{\partial y^2} (\cos^2 \theta + \sin^2 \theta) \]

\[ = \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{1}{r^2} \frac{\partial^2 c}{\partial \theta^2} \quad (3.20) \]

Assume radial symmetry, then:

\[ \nabla \cdot \nabla c = \frac{Q}{2\pi r} \frac{\partial c}{\partial r} \]

\[ \frac{\partial c}{\partial \theta} = \frac{\partial^2 c}{\partial \theta^2} = 0 \]

and Eq. 3.19 can be replaced by an equation in a single spatial variable \( r \):

\[ \frac{\partial c}{\partial t} = \frac{\partial}{\partial r} \left( nrD_m \frac{\partial c}{\partial r} + \frac{Q}{2\pi} \frac{\partial c}{\partial r} \right) - \frac{Q}{2\pi} = 0 \quad (3.21) \]

where the early time \( t_r \) is given and the front does not reach distance \( R \) from the well by time \( t_r \). The time \( t_r \) is usually initialized to 0.01 pore volume injected. Although the analytical solution to Eq. 3.21 exists, its use is not computationally attractive. The Galerkin finite element with the backward difference in time is used to solve Eq. 3.21.
In order to continue the time stepping from the radial solution to the regular tensor product space, a least-square projection is used:
Let \( c^{tr} = \) projected concentration
\( c^* = \) radial concentration

Then the orthogonal projection is defined as:
\[
\int_\Omega (c^{tr} - c^*)V = 0 \tag{3.22}
\]
where \( V \) is a bilinear test function. Eq. 3.22 projects \( c^* \) onto the orthogonal complement to \( c^{tr} \).

3.3 HYDRAULICS OF GROUNDWATER FLOW

The computed fluid velocities help to determine the time-stepping procedure in the characteristic-based method and since accurate velocities are crucial in the method's ability to conserve mass, very accurate Darcy velocities are necessary. Mixed finite element (Darlow et. al., 1982; Douglas et. al., 1983; Ewing et. al., 1983; Russell and Wheeler, 1983) is used to solve for the head and the Darcy velocity simultaneously, as a system of first order partial differential equations, rather than the usual single elliptic equation for the head and then differentiating the head values to find the velocity. It is an elementary consequence of approximation theory that one order of convergence is lost in passing from head to velocity by differentiating. The first order system for groundwater hydraulics is:
\[ V = -k \cdot \nabla h, \quad (x,y) \in \Omega = (0, I \times 0, J) \quad (3.23) \]
\[
\nabla \cdot (b \cdot V) = Q, \quad (x,y) \in \Omega = (0, I \times 0, J) \quad (3.24) \]
\[
h(x,0) = g_0, \quad (g_0 < g_1) \quad (3.25) \\
h(x,J) = g_1, \quad (g_0 < g_1) \\
\nabla \cdot \nabla h = 0, \quad y \in (0,J); y \in (I,J) \quad (3.26) \\
\]

where

\[ V = \text{Darcy velocity} \]
\[ k = \text{hydraulic conductivity tensor} \]
\[ b = \text{aquifer thickness} \]
\[ h = \text{hydraulic head} \]
\[ Q = \text{point sources and sinks (Dirac measure)} \]

In these equations \( b \) is the actual constant aquifer thickness for a confined or semi-confined aquifer, while for an unconfined aquifer, \( b = h - B \), where \( B \) is the elevation of the base of the aquifer. Eqs. 3.23 and 3.24 are solved simultaneously along with specified head and fluxes around the boundary of the domain.

3.3.1 Formulation of the Mixed Finite Element Method

Before proceeding to the mathematical formulation of the mixed method, it is necessary to define some notation.

Denote:

\[
(u,w) = \int_{\Omega} (u \cdot w) \, d\omega \\
<u,w> = \int_{\partial \Omega} (u \cdot w) \, dR
\]
where \( \cdot \) is the dot product. Let \( H(\text{div}, \Omega) \) be the set of vector functions \( u \in [L^2(\Omega)]^2 \) such that \( \nabla \cdot u \in L^2(\Omega) \), where \( L^2(\Omega) = \{ \| e \|_{L^2} = (\int_\Omega (e^2 \, dx)^{1/2} \} \) is the mean-square norm, and let \( U \in H(\text{div}, \Omega), \, w \in L^2(\Omega) \).

Multiplying Eq. 3.23 by \( k^{-1}u \), \( u \in U \), integrating, and integrating by parts to obtain:

\[
(k^{-1}v, u) = -(\nabla h, u) = (h, \nabla \cdot u) - \langle h, u \cdot \eta \rangle, \quad u \in U
\]

Thus

\[
(k^{-1}v_x, u_x) + (k^{-1}v_y, u_y) = \frac{\partial y}{\partial x} \frac{\partial u}{\partial y} + \frac{\partial y}{\partial x}
\]

\[
= \int_0^I [ -g_0(x)u_y(x, 0) + g_1(x)u_y(x, i) ] \, dx, \quad u \in U
\]

where \( v_x, v_y \) represent velocities in \( x \) and \( y \) directions, respectively, and \( u_y \) refers to the test function in the \( y \) direction. Assume the aquifer thickness is constant and divide both sides of Eq. 3.24 by \( b \) to obtain

\[
\nabla \cdot V = Q/b = q
\]

Multiply Eq. 3.29 by \( w \in W \) and integrate to obtain

\[
(\nabla \cdot V, w) = (q, w), \quad w \in W
\]

Equivalently

\[
(v_x, v_y, w) = (q, w)
\]

The system 3.28 and 3.31 is then approximated by finite elements. For suitable finite dimensional subspaces \( U_h \in U \) and \( W_h \in W \) to be described next, the approximation is

\[
(\nabla_h, h_h) \in U_h \times W_h \text{ satisfying}
\]
\[(k^{-1}v_h^x, u^x) + (k^{-1}v_h^y, u^y) = \frac{\partial u}{\partial x} - \frac{\partial u}{\partial y}\]

\[= \int_0^1 [-g_0(x)u^y(x, 0) + g_1(x)u^y(x, 1)]dx, \quad u \in \overline{U}_h \quad (3.32)\]

\[(V_{hx}^x + V_{hy}^y, w) = (q, w), \quad w \in \tilde{W}_h \quad (3.33)\]

The finite dimensional subspaces need certain properties in order for the convergence analysis of Breeze, Falk and Osborn and Raviart and Thomas (1977) to hold. One of these is that \( \text{div}(U_h) \subseteq W_h \).

3.3.2 Raviart-Thomas Space

The space \( M_k(r, \Delta x) \) was defined in section 3.5; it is repeated here.

\[M_k(r, \Delta x) = \{ \psi \in C^k([0, c]): \psi \text{ is a polynomial of degree } \leq r \text{ on each subinterval } \Delta x \}\]

when \( k = -1 \) refers to the discontinuous functions.

Let \( W_h = M_k(m, \Delta x) \otimes M_k(m, \Delta y) \),

\[U_h = M_{k+1}(m+1, \Delta x) \otimes M_k(m, \Delta y) \times M_k(m, \Delta x) \otimes M_{k+1}(m+1, \Delta y) \]

and \( \tilde{U}_h = M_{k+1}(m+1, \Delta x) \otimes M_k(m, \Delta y) \times M_k(m, \Delta x) \otimes M_{k+1}(m+1, \Delta y) \)

where \( \otimes \) is tensor product, and these are known as the Raviart-Thomas finite dimensional subspaces. Examples of Raviart-Thomas subspaces:

\[M_{-1}(0, \Delta x) = \text{discontinuous constants on } \Delta x\]

\[M_{-1}(1, \Delta x) = \text{discontinuous linears on } \Delta x\]

\[M_0(1, \Delta x) = \text{continuous linears on } \Delta x\]

\[M_0(2, \Delta x) = \text{continuous quadratics on } \Delta x\]
The Raviart-Thomas subspaces are used because they satisfy the minimum continuity requirement for $V_h$ and $W_h$. The following will focus on the development of the next to lowest-order Raviart-Thomas subspaces since the computer code is based on this order.

For the next to lowest order Raviart-Thomas subspace, $k=-1$ and $m=1$, $W_h$ and $U_h$ become:

$$W_h = \mathcal{M}_{-1}(1,\Delta x) \otimes \mathcal{M}_{-1}(1,\Delta y)$$

$$U_h = \mathcal{M}_{0}(2,\Delta x) \otimes \mathcal{M}_{-1}(1,\Delta y) \times \mathcal{M}_{-1}(1,\Delta x) \otimes \mathcal{M}_{0}(2,\Delta y)$$

Let $\psi_{ij}$ denote bases for $W_h$ and

$$\psi_{ij} = W_i(x)W_j(y), \quad i=1,\ldots,2Nx; \quad j=1,\ldots,2Ny$$

where $W_i(x)$ and $W_j(y)$ are linear functions that their values are unity at one Gauss point and zero at all other Gauss points. Specifically, if $\sigma_1$ and $\sigma_2$ are two Gauss points defined on $[x_{i+1},x_i]$ along the $x$-coordinate, then:

$$W_{2i-1}(x) = \frac{x_{i-1} + \sigma_2(x_i-x_{i-1}) - x}{(\sigma_2-\sigma_1)(x_i-x_{i-1})}, \quad x \in [x_{i-1},x_i]$$

$$W_{2i}(x) = \frac{x - \sigma_1(x_i-x_{i-1}) - x_{i-1}}{(\sigma_2-\sigma_1)(x_i-x_{i-1})}, \quad x \in [x_{i-1},x_i]$$

Figure 3.3 shows the basis functions $W_i(x)$. The $W_j(y)$ are defined similarly. Any $W \in W_h$ can therefore be written as

$$W = \sum_{j=1}^{2Ny} \sum_{i=1}^{2Nx} \alpha_{ij} W_i(x)W_j(y)$$

where the $\alpha_{ij}$ are constant.

The basis functions for $U_h$ are $\Phi_{ij}(x,y)$, where $\ell = 1,2$ indexes the $x$ and $y$ direction velocities respectively and
FIGURE 3.3 Basis Function for $W_i(x)$.
\[ \phi_{ij} = \begin{cases} V_i(x)W_j(y) & , \quad i = 1, \ldots, 2N_x \\ 0 & , \quad j = 1, \ldots, 2N_y \end{cases} \]

and

\[ \phi_{ij} = \begin{cases} 0 & , \quad i = 1, \ldots, 2N_x \\ V_j(x)W_i(x) & , \quad j = 1, \ldots, 2N_y \end{cases} \]

where \( W_i(x) \) and \( W_j(y) \) are defined as for \( W_n \) and

\[ V_{2i-1}(x) = \begin{cases} \frac{4(x-x_{i-1})(x_i-x)}{(x_i-x_{i-1})^2} & , \quad x \in [x_{i-1}, x_i] \\ 0 & , \quad \text{otherwise} \end{cases} \]

and

\[ V_{2i}(x) = \begin{cases} \frac{(x-x_{i-1})}{(x_i-x_{i-1})} & , \quad x \in [x_{i-1}, x_i] \\ \frac{(x_{i+1}-x)}{(x_{i+1}-x_i)} & , \quad x \in [x_i, x_{i+1}] \\ 0 & , \quad \text{otherwise} \end{cases} \]

\[ V_{2j-1}(y) = V_{2i}(x) \quad , \quad V_{2j}(y) = V_{2i-1}(x) \]

Figure 3.4 shows the basis function for \( V_j(y) \). Any \( V \in U_h \) can be written as

\[ v^x = \sum_{i=1}^{2N_x-1} \sum_{i=1}^{2N_y} [ \beta_{ij} V_j(x) V_i(y) ] \quad (3.35) \]

and

\[ v^y = \sum_{i=1}^{2N_x} \sum_{i=1}^{2N_y+1} [ \beta_{ij} V_j(y) W_i(x) ] \quad (3.36) \]
FIGURE 3.4. Basis Function for $V_j(y)$
3.3.3 Algebraic System

Using the basis functions expressed in equations 3.33 - 3.36, equations 3.32 - 3.33 can be written in matrix form.

\[
\begin{bmatrix}
    M_1 & 0 & -N_1 \\
    0 & M_2 & -N_2 \\
    N_1^T & N_2^T & 0
\end{bmatrix}
\begin{bmatrix}
    \beta^2 \\
    \beta^2 \\
    \alpha
\end{bmatrix}
= \begin{bmatrix}
    0 \\
    RR \\
    RHS
\end{bmatrix}
\]

where

\[
M_1 = \begin{bmatrix}
    M_{11} & M_{12} \\
    & \ddots \\
    & & M_{1,2Ny}
\end{bmatrix}
\]

Each \( M_{1k} \) is a tridiagonal matrix of order \( 2N_x-1 \) and is determined by:

\[
M_{1k} = \iint_{\Omega} \kappa^{-1} v_i(x)w_j(y)v_m(x)w_n(y) \, dx \, dy
\]  

(3.38)

and

\[
M_2 = \begin{bmatrix}
    M_{21} & M_{22} \\
    & \ddots \\
    & & M_{2,2Ny}
\end{bmatrix}
\]

Each \( M_{2k} \) is also a tridiagonal matrix of order \( 2Ny+1 \) and is determined by:

\[
M_{2k} = \iint_{\Omega} \kappa^{-1} v_j(y)w_i(x)v_n(y)w_m(x) \, dx \, dy
\]  

(3.40)

and

\[
N_1 = \begin{bmatrix}
    n_{11} & n_{12} \\
    & \ddots \\
    & & n_{1,2Ny}
\end{bmatrix}
\]

Each \( n_{1k} \) is determined by
\[ n_{1k} = \int \int_{\Omega} W_i(x) W_j(y) V_m'(x) W_n(y) \, dx \, dy \]  
(3.42)

and
\[
N_2 = \begin{bmatrix}
  n_{21} \\
  n_{22} \\
  \vdots \\
  n_{2,2N_2}
\end{bmatrix}.
\]  
(3.43)

Each \( n_{2k} \) is determined by
\[ n_{2k} = \int \int_{\Omega} W_j(x) W_i(y) V_m'(y) W_m(x) \, dx \, dy \]  
(3.44)

The matrix \( N_1 \) is of size \((2N_x-1)2N_y \times 2N_x 2N_y\) while \( N_2 \) is of size \((2N_y+1)2N_x \times 2N_x 2N_y\). Although \( N_1 \) is not square, it has essentially a block diagonal form. \( N_2 \) can be made to have the same form by permuting the rows and corresponding columns.

The right hand side of the system 3.37 has two non-zero vectors, they are:
\[
RR = \int_0^1 [-g_0(x)u^2(x,0)+g_1(x)u^2(x,J)] \, dx
\]  
(3.45)

and
\[ \text{RHS} = \int \int_{\Omega} [qW_i(x)W_j(y)] \, dx \, dy \]  
(3.46)

Eliminating \( \beta^1 \) and \( \beta^2 \) from the system 3.37 yields a system for \( \alpha \) given by:
\[
M_1 \beta^1 - N_1 \alpha = 0 \quad \Rightarrow \quad \beta^1 = M_1^{-1}N_1 \alpha
\]  
(3.47)

\[
M_2 \beta^2 - N_2 \alpha = RR \quad \Rightarrow \quad \beta^2 = M_2^{-1}(N_2 \alpha + RR)
\]  
(3.48)

\[
N_1^t \beta^1 + N_2^t \beta^2 = \text{RHS}
\]
\[
\Rightarrow N_1^t(M_1^{-1}N_1 \alpha) + N_2^t(M_2^{-1}(N_2 \alpha + RR)) = \text{RHS}
\]
\[
\Rightarrow (N_1^t M_1^{-1} N_1 + N_2^t M_2^{-1} N_2) \alpha = \text{RHS} - N_2^t M_2^{-1} RR
\]  
(3.49)
Then solve for $a$ using preconditioned conjugate gradient methods. Once $a$ has been computed, $b$ can be determined by solving

$$
\begin{bmatrix}
M_1 & 0 \\
0 & M_2
\end{bmatrix}
\begin{bmatrix}
b^1 \\
b^2
\end{bmatrix}
= 
\begin{bmatrix}
N_1a \\
RR + N_2a
\end{bmatrix}
$$

(3.50)

3.4 **PRECONDITIONED CONJUGATE GRADIENT METHODS**

The method of conjugate gradient has been known for some time, having been developed independently by Hestenes and Stiefel (1952) with the cooperation of Rosser, Forsythe and Page, but it has received little attention until recently. One of the most important reasons for the popularity of the conjugate gradient method as a practical method is the elimination of manually estimating parameters, required for other iterative solvers. The conjugate gradient algorithm is equivalent to finding the minimizer of a quadratic functional

$$f(x) = 1/2(x^TAX) - b^Tx$$

with a positive definite Hessian $A$ and right hand side vector $b$. Unlike the method of steepest descent, it has the property of yielding the exact solutions (in the absence of rounding errors) after at most $N$ iterations, where $N$ is the order of $A$. By performing iterations of the type

$$x^{k+1} = x^k + \tau_kd^k \quad , \quad k = 0,1,2,\ldots$$

where $d^k$ is the search direction and $\tau_k$ has the property of minimizing the function $f(x + \tau_kd^k)$, it also makes gradient
at $x^{k+1}$ orthogonal to search direction $d^k$. It has been shown that the number of iterations necessary to make the error less than $\epsilon$ times the initial error is roughly bounded by $1/2(\sqrt{S(A)}) \ln(2/\epsilon)$, where $S(A)$ is the spectral condition number of $A$, equal to the ratio of the largest and smallest eigenvalues of $A$ [Axelsson and Barker, in press]. Concisely et. al. also introduced the concept of preconditioning, a technique for accelerating the rate of convergence. Preconditioning requires one to choose a positive definite matrix $C$ (the so-called "preconditioning matrix"). The rate of convergence for the conjugate gradient method in its preconditioned form is bounded by a constant times the square root of rate of the largest smallest eigenvalue of $C^{-1}A$.

The main advantage of using the preconditioned conjugate gradient algorithm (PCG) over other iterative procedures is that it is not necessary to define acceleration parameters. Moreover, storage requirements for PCG are substantially less than for direct method. For the non-steady state problem, one has a good initial guess for the approximate solution. This and the simplicity of implementation are two advantages of the PCG method over iterative, multi-grid methods. The following will present the computer algorithm for the preconditioned conjugate gradient procedure:

\begin{align*}
(1) \quad \tau_k &= \frac{q^k h^k}{d^k t d^k} \\
(2) \quad x^{k+1} &= x^k + \tau_k d^k
\end{align*}
\( q^{k+1} = q^k + \tau_k Aq^k \)

(4) \( h^{k+1} = c^{-1}q^k \theta^{k+1} \)

(5) \( \beta^k = \frac{q^{k+1} \theta^{k+1}}{q^k \theta^k} \)

(6) \( \Delta^{k+1} = -h^{k+1} + \beta_k \Delta^k \)

Initially choose \( x^0 \) and put \( g^0 = Ax^0 - b \), \( h^0 = c^{-1}g^0 \) and \( \Delta^0 = -h^0 \). The multiplication by \( C^{-1} \) in (4) is to be interpreted as solving a system of equations with coefficient matrix \( C \).

### 3.5 Boundary Conditions

During the early development of the modified method of characteristics, \((\text{Eq. 3.16} - 3.18)\), a no flow boundary condition was assumed for all four boundaries. To allow simulation of more realistic field conditions, a mixed boundary condition with two no flow boundaries and with two specified head boundaries was incorporated into the variational form of the groundwater flow equation. Since \(\text{Eq. 3.18} \) was written for the no flow condition it is inconsistent with a specified hydraulic head boundary. A specified head generates mass fluxes through the boundary if the contaminated plume crosses the boundary. Therefore, a second equation which calculates mass fluxes through the boundary must be included in the transport process. However, if the contaminated plume is at a distance to the boundary, then the no-flow condition for the mass transport
is acceptable. The no-flow condition is also an acceptable approximation if one only accounts for the advective flux but not the diffusive flux through the boundary. The mathematical description of this approximation is given as follows.

Multiply Eq. 3.4 by a test function \( u \), integrate over the spatial domain, integrate by parts to obtain:

\[
\begin{align*}
\frac{\partial c}{\partial t} \int_{\Omega} b(n+\rho F') - u dx dy + \int_{\Omega} b \vec{V} c \vec{V} u dx dy - \int_{\Omega} b \vec{V} c \vec{V} u dx dy \\
- \int_{\partial \Omega} b \vec{V} c \vec{N} u ds + \int_{\partial \Omega} b \vec{V} u \vec{N} ds
\end{align*}
\]

\[
= \int_{\partial \Omega} b \vec{V} c \vec{N} u ds + \int_{\partial \Omega} b \vec{V} u \vec{N} ds
\]

\[
= \int_{\partial \Omega} b c \vec{N} u ds
\]

(3.51)

If the test function \( u = 1 \), then Eq. 3.51 becomes:

\[
\begin{align*}
\int_{\Omega} b(n+\rho F') - dx dy + \int_{\partial \Omega} b \vec{V} c \vec{N} ds + \int_{\partial \Omega} b \vec{V} c \vec{N} ds
\end{align*}
\]

\[
= \int_{\partial \Omega} b c \vec{N} ds
\]

(3.52)

The first term in the left hand side represents the accumulation of mass, the second term is the diffusive flux normal to the boundary, and the third term is the advective flux normal to the boundary; the right hand side is the point source and sink term. Eq. 3.52 states the time rate of increase of mass within a domain is just equal to the net rate of mass inflow to the domain. If the contaminated plume is initially within the boundary of the problem, then the two boundary integral terms of Eq. 3.52 represent outward flux normal to the boundary. In the development of
the modified method of characteristics the boundary
condition for the transport equation was specified as:

∇c·\vec{n} = 0

From Eq. 3.52 this boundary condition states that the
diffusive flux is negligible and it considers only the
advective flux across the boundary. Although this is not
correct for the boundaries with specified hydraulic heads of
the groundwater flow equation, however, the no-diffusive-
flux condition is a reasonably good approximation and is
physically plausible if the contaminated plume is contained
within the boundary.

3.6 SUMMARY

In summary, the modified method of characteristics has
shown theoretically that much larger time steps can be used
with no loss of accuracy. Other advantages of the method
include no numerical dispersion, grid orientation, or
numerical oscillation problems. These problems present
serious numerical errors that are commonly shared by many
other numerical methods. In addition, the Darcy velocity is
simulated very accurately and efficiently by the mixed
finite element procedure which adds to the overall
advantages of the computer program. The overall flow chart
of the computer program that simulates both the transport
equation and the groundwater hydraulics is given in Appendix
III.
CHAPTER FOUR
MODEL VERIFICATION AND APPLICATION

To test the computational accuracy, comparisons between
the numerical solution and analytical solutions provide
useful verifications. This comparison is a first step in
the numerical modeling of physical systems. Two
representative analytical solutions were used to test the
MMOC method in this chapter. The first solution involves a
single injection well and the second involves an injection-
pumping pair.

The reliability of predictions produced by deterministic
mathematical models is limited by the completeness of the
data base describing a physical system and by the stochastic
nature of some parameters. Therefore, the linkage between a
deterministic mathematical model and stochastic input of
parameters produces possible range of predictions. In many
cases, this linkage must be iterated back and forth several
times, that is, conditioned on field measurements.

This chapter discusses the Turning Bands Method (TBM)
that simulates random hydraulic conductivity fields. These
random hydraulic conductivity fields are input to the MMOC
method and results are presented in relative concentration
contours. Variations in hydraulic conductivity fields
produce a marked change in both the shape of the plume and
the distribution of concentration within the plume. With
measured data in several points of a particular field site,
several statistical parameters (e.g. correlation coefficient, covariance function) of the hydraulic conductivity simulation can be adjusted to fit observed data. This stage is usually called sensitivity analyses and is an important process in examining the reliability of numerical modeling. There are, of course, other parameters which would affect the shape of the simulated plume. These parameters include the dispersivity, hydraulic gradient, loading capacity, and the orientation of the grid. In field applications, these parameters often are not well defined and therefore add to the complexity of the modeling.

4.1 COMPARISON WITH SINGLE WELL ANALYTICAL SOLUTION

For a continuous injection of constant mass per unit length, \( f_m'\) at an injection well, the analytical solution to the transport equation (Eq. 3.5) with uniform steady flow in the \( x\) direction was given by Wilson and Miller (1978).

\[
C = \frac{f_m' \exp(x/B)}{4\pi n(D_x D_y)^{1/2}} W(u, r/B)
\]

(4.1)

where

\( C \) = concentration of the substance in solution
\( B \) = \( 2D_x/V \)
\( u \) = \( r^2/4D_x t \)
\( r \) = \( \left| x^2 + \frac{D_x}{D_y} y^2 \right|^{1/2} \)
\( D_x = \alpha_x V \) = longitudinal dispersion coefficient
\( D_y = \alpha_y V \) = transverse dispersion coefficient
n = porosity

$\alpha_x, \alpha_y = \text{dispersivities in the } x-\text{ and } y-\text{ directions, respectively}$

\[ W(u, r/B) = \int_0^\infty \frac{1}{u} \exp[-(\theta + r^2/4B^2\theta)] d\theta \]

in which $W(u, r/B)$ is the "well function" derived by Hantush (1956). The function $r$ is a weighted distance, or radius, from the source to the point of interest. The coefficient $B$ is mixing scale factors equivalent to the Hantush leakage factors. For large $r/B$, Wilson and Miller (1978) used the Laplace's method to approximate the Hantush well function. The final form of the approximated solution is given as

\[ W(u, r/B) = \frac{\pi B}{2r} \frac{1/2 \exp(-r/B)}{\text{ERFC} - \left(\frac{r/B - 2u}{2u^{1/2}}\right)} \quad (4.2) \]

where ERFC = complementary error function. This expression for $W(u, r/B)$ is reasonably accurate (within 10%) for $r/B > 1$ and very accurate (within 1%) for $r/B > 10$.

The solution was used to study the Long Island industrial waste site described by Perlmutter and Lieber (1970) and Pinter (1973). Good agreement between the measured extent of the contaminated plume and the predicted analytical solution was reported in Wilson and Miller (1978). For a direct comparison with the numerical model, a FORTRAN program was written based on the analytical solution (Appendix I). The major inputs to the analytical solution are mass rate of injection, dispersivities in $x$- and $y$-directions, and a one-dimensional areal uniform flow field.
In order to produce the same one-dimensional areal uniform flow field in the numerical simulation, the hydraulic heads on the two opposite boundaries along the flow direction were specified as two different constant heads. Both models were simulated on the CRAY-XMP supercomputer with the following parameters:

\[
K = 78.6 \text{ Darcy (2.49} \times 10^{-3} \text{ ft/sec)}
\]

\[
t = 2800 \text{ days}
\]

\[
\alpha_x = 69.9 \text{ ft}
\]

\[
\alpha_y = 14.0 \text{ ft}
\]

\[
n = 0.35
\]

\[
f_m' = 52 \text{ lb/day}
\]

Solution matrices resulting from computer simulations at 2800 days after initial injection were downloaded to an IBM-PC through communication programs. These solution matrices were then plotted as concentration contours. Figures 4.1 and 4.2 show the concentration contour maps for the analytical solution and the numerical simulation respectively. Excellent agreement at a small distance downstream from the injection well was shown. Around the injection well, the concentration contours simulated by the numerical model spread wider in the transverse direction than the one produced by the analytical solution. The analytical solution treats the injection well as a constant rate of mass influx without any head build-up associated with the pumpage of fluids, which is an approximation to the
Concentration Contours
Long Island, NY Plume
2800 days after injection

FIGURE 4.1
ANALYTICAL SOLUTION
(Wilson and Miller)
Concentration Contours
Long Island, NY Plume
2800 days after injection

FIGURE 4.2
NUMERICAL SOLUTION
(MMOC)
observed physical phenomenon. While the numerical model considered the head build-up from the injection of fluids, therefore a faster flow rate near the injection well is simulated, and the wider dispersion in the transverse direction is a direct consequence of the faster flow rate.

4.2 COMPARISON WITH AN INJECTION-PUMPING WELL PAIR
ANALYTICAL SOLUTION AND THE USGS SOLUTE TRANSPORT MODEL

As a second test of model accuracy, an analytical solution that involves an injection-pumping well pair was and compared with both the modified method of characteristics and the USGS solute transport model. The analytical solution was developed by Grove and Beetem (1971) of the USGS for the purpose of evaluating an aquifer's porosity and longitudinal dispersivity. In the solution, the flow pattern between wells is divided into a number of crescents (Figure 4.3) through which the water is assumed to pass. Each crescent is treated as a laboratory column of length L, and by means of suitable dispersion equation the breakthrough curve for this column or crescent is calculated. In a similar manner, the breakthrough curve can be calculated for all the crescents comprising the flow field, the flow can be added, and a composite breakthrough curve for a particular dispersion coefficient can be prepared.
FIGURE 4.3 Flow Pattern Between Wells
(from Grove and Beets, 1971)
The length of a streamline arc, $L$, between two wells was obtained by line integration of the streamline equation. Without detailed descriptions of the derivation, the final equation of the arc length of the streamline is given as

$$
L = \frac{2\alpha a}{\sin \alpha}
$$

where $2a$ is the distance between wells, and $\alpha = \pi + 2\pi \psi / q$ in which $q$ is the pumping rate and $\psi$ is the streamline equation:

$$
\psi = \frac{q}{2\pi} \tan^{-1} \frac{2ay}{a^2-x^2-y^2}
$$

The time for a water particle to travel along a particular streamline is:

$$
t = \frac{4\pi na^2}{q \sin^2 \alpha} [\cot \alpha - 1]
$$

where $n$ is the porosity of an aquifer.

To derive the relative concentration of the tracer material at the pumping well, the travel time, $t$, and the arc length, $L$, are combined with a solution to the one-dimensional advection-dispersion equation for a column of fixed length. The final approximated form of the breakthrough curve at the pumping well is:

$$
\frac{C}{C_0} = 0.5 \text{ERFC}[(P/t')^{1/2}(1-t')]
$$

$$
+ (4Pt'/\pi)^{1/2} [3 + 2P(1 + t')]
$$

$$
- \exp[-P(1 - t')^2/t']
$$

$$
- [0.5 + 2P(3 + 4t') + 4P^2(1 + t')^2]
$$

$$
x \exp(4P)\text{ERFC}[(P/t')^{1/2}(1+t')]
$$

(4.6)
in which \( P \) is the Peclet number, and \( t' \) is equal to \( T/t \)
where \( T \) is the time of interest and \( t \) is the travel time
between wells. A FORTRAN code was written based on this
solution and is given in Appendix II.

In order to compare with the analytical solution the
distance between wells, the pumping rate, and the size of
domain must be carefully designed in the numerical
simulations so that there is no boundary effect on the
numerical solutions. The distance between two wells was set
to equal 6 ft in a 30 \( \times \) 30 ft domain and the pumping rate
was equal to 1.5 ft\(^3\)/day-ft. The porosity of the aquifer
was 0.3 and the longitudinal dispersivity was equal to 0.7
ft.

Two groups of numerical simulations were made, the first
group was simulated on a 30 \( \times \) 30 grid system for both of the
USGS solute transport model and the MMOC method, and the
second group was simulated on a more refined 60 \( \times \) 60 grid
system. One of the advantages of the MMOC method is that
grid points are not required to be uniformly spaced, while
the USGS solute transport model requires uniform grids. For
a nonuniform grid system, more refined grids can be placed
around wells which are singular points, and therefore more
accurate simulations can be achieved.

Figure 4.4 shows breakthrough curves from the analytical
solution and from the two numerical models on the 30 \( \times \) 30
grid system. Excellent agreement between the MMOC and the
FIGURE 4.4 Comparison of the MMOC model, the USGS model, and the Analytical Solution
30 x 30 grid system
analytical solution is shown. The breakthrough curve from the USGS solute transport model deviates a distance from the analytical solution and oscillates between time steps.

Figure 4.5 shows three other breakthrough curves for the 60 x 60 grid system. Again, the solution from the MMOC method agrees better with the analytical solution than the USGS model does. The time step of the concentration calculation on the 60 x 60 grid system was 0.85 hours for the USGS model, which was calculated internally in the computer program due to the Courant number restriction, while the iteration time step for the MMOC method was set to equal 2.4 hours which is approximately three times larger than the time step from the USGS model.

4.3 CONVERGENCE STUDY

To prove that even larger time steps can be taken without sacrificing much of the solution's accuracy, two more computer runs were simulated on the 60 x 60 grid system with time steps equal to 4.8 and 12 hours respectively. Figure 4.6 shows breakthrough curves from the 2.4 hours, 4.8 hours, and 12 hours time step simulations. These three curves are very close at early times and deviate a small distance from the 2.4 hours simulation at later times, which matches the analytical solution exactly. At 16 days after initial injection there is only a 3% difference between the 12 hours and the 2.4 hours simulations, while there is a 9%
FIGURE 4.5 Comparison of the MMOC model, the USGS model, and the Analytical Solution 60 x 60 grid system
Figure 4.6 Time Step Convergence Study (MMOC)
difference between the 12 hours and the 2.4 hours simulations. Consider the inherent variability in several aquifer's parameters; e.g., porosity and hydraulic conductivity, a 9% error in some cases may be tolerable as a preliminary investigation of a contaminated site. This result demonstrates the theoretical proof (Douglas and Russell, 1982) that much larger time steps can be taken in the MMOC method than other standard finite element or finite difference methods.

A grid-refinement convergence study is also experimented with the MMOC model. In this experiment, the 30 ft × 30 ft domain was divided into 30 × 30, 60 × 60, and 120 × 120 grid systems. Input parameters were:

- Diffusion coefficient = 0.15 ft²/day
- Longitudinal dispersivity = 0.30 ft
- Transverse dispersivity = 0.003 ft
- Porosity = 0.10
- Permeability = 0.5 Darcy
- Q = 3 ft³/day-ft

Injection well and pumping wells were placed along a diagonal of the domain and were separated with a distance of 25.45 ft. Figure 4.7 shows breakthrough curves at the pumping well from these three simulations. Figures 4.8 and 4.9 show the relative concentration contour maps of the 30 × 30 and 60 × 60 grid system simulations, respectively. Breakthrough curves are almost identical from the
FIGURE 4.8  Grid Size Convergence Study
30 x 30 grid system
FIGURE 4.9  Grid Size Convergence Study
60 x 60 grid system
simulations on the $60 \times 60$ and the $120 \times 120$ grid systems. A 6\% difference between the $30 \times 30$ and the $60 \times 60$ simulations is shown at the end of 20 days. In general, the MMOC method requires a fairly fine grid system as in other standard finite element methods in order to resolve a sharp front or to obtain accurate resolutions.

4.4 ADVECTIVE-DOMINATED SIMULATIONS

To test the code's ability in handling sharp fronts, experiments which varied the Peclet number ($P_e$) from 10 to 1000 were performed. In these experiments, the following parameters were used in a $30 \text{ ft} \times 30 \text{ ft}$ domain:

\begin{align*}
Q &= 5 \text{ ft}^3/\text{day-ft} \\
\alpha_L &= \text{from 0.03 ft to 3 ft} \\
\alpha_T &= \text{from 0.003 ft to 0.3 ft} \\
D^* &= 0 \\
n &= 0.1 \\
k &= 0.5 \text{ Darcy}
\end{align*}

Runs made with $P_e = 10$, $P_e = 100$, and $P_e = 1000$ are shown in Figures 4.10, 4.11, and 4.12, respectively. The time step was taken to be 0.48 hours with a grid system of $60 \times 60$ intervals. It is obvious from those figures that the contour lines are spread much wider and therefore more dispersive from the run of $P_e = 10$ than the runs of $P_e = 100$ and $P_e = 1000$. The distance between the points $C/C_0 = 0.9$ and $C/C_0 = 0.3$ of the $P_e = 10$ run is about 7.2 times as wide.
 FIGURE 4.10  Peclet Number 10
FIGURE 4.11  Peclet Number 100
FIGURE 4.12  Peclet Number 1000
as the $P_e = 1000$ run. No oscillation, overshoot, or numerical dispersion was observed in the $P_e = 1000$ run, a highly advective-dominated case.

4.5 ADSORPTION SIMULATIONS

To illustrate the influence of adsorption as a concentration-altering mechanism, a retardation factor of 1.2 was tested on a 60 x 60 grid system in the 30 ft x 30 ft domain. Figure 4.13 compares a non-retarded breakthrough curve at the pumping well with a 20% retarded curve. Figure 4.14 shows the relative concentration contours of the 20% retardation simulation with a retardation factor of only 1.2, a 40% reduction of the concentration at the end of 20 days after initial injection was simulated. The MMOC method was further simulated with a retardation factor of 2.0. The plume was almost completely retarded for this case. At the end of 20 days after injection, the relative concentration at the pumping well was only 2% of the original tracer versus 47% of the non-retarded case.

4.6 SIMULATIONS ON RANDOM HYDRAULIC CONDUCTIVITY FIELDS

To further test the flexibility of the model, the model was tested against a random hydraulic conductivity field generated through the Turning Bands Method. The Turning Bands Method (TBM) was originally introduced by G. Matheron
FIGURE 4.13 Effect of Retardation
60 x 80 grid system
FIGURE 4.14  20% Adsorption
(1973) of the Ecole des Mines de Paris. The method was used primarily to account for uncertainties introduced by the unpredictable nature of the process or by the scariness of measurements. In groundwater models, the random hydraulic conductivity fields can be obtained based on conditional TBM simulations, that is simulations which preserve the observed values at the data points.

Prior to the discussion of the TBM, the Monte Carlo simulations will be introduced. The Monte Carlo simulations refers to a set of repetitive simulations with a mathematical model and the associated statistical analysis of the results. In the groundwater flow simulations, if the probability density function (pdf) for hydraulic conductivity is known, then the distribution of hydraulic heads at any point can be analyzed statistically (Freeze, 1975). Suppose the pdf for hydraulic conductivity, $k$, is log normal distributed, which was supported by a large body of direct evidence (Law, 1944; Bulnes, 1946; Warren et. al., 1961), then the random variable

$$ y = \log k $$

is normal. The normal generator is

$$ y = \sigma_y R_N + \mu_y $$

where $R_N$ is a random number taken from $N[0,1]$, $\mu_y$ is the mean, and $\sigma_y$ is the standard deviation. Since $y = \log k$, then $k = e^{2.3y}$, and the log normal generator for $k$ is

$$ k = \exp[2.3(\sigma_y R_N + \mu_y)] $$
For any spatial distribution of k values chosen in the foregoing way, a special hydraulic head distribution can be determined based on Eq. 3.21 and Eq. 3.22. If one carries out such an analysis for a number of Monte Carlo runs, the distribution of hydraulic head at any point can be analyzed statistically.

The Monte Carlo method requires a number of simulations to analyze the statistics of a field, which can be computationally costly. The TBM simulates possible realizations of the underlying random fields by only one simulation. Instead of simulating the two- or three-dimensional field directly, the TBM transforms the higher dimensional simulation to a unidimensional one. The results of several lines simulations are added to generate the point value of the two- or three-dimensional field (Figure 4.15). Through this transformation the cost of simulation increases proportionally to the square root of the number points in the field at which one generates.

In Figure 4.15, O is an arbitrary origin and generates lines with random direction in two or three dimensions. Let \( i \) be one of those lines, forming an angle \( \theta \) with the x-axis. Along each line \( i \), generate a unidimensional process having zero mean and covariance function \( C_1(\tau) \), where \( \tau \) is the coordinate along line \( i \). The function \( C_1(\tau) \) was derived as a function of two-dimensional covariance function by Mantoglou and Wilson (1981). Any point in a two-dimensional
FIGURE 4.15 Schematic Representation of the Field and the Turning Bands Lines (from Mantoglou and Wilson, 1981)
field can be orthogonally projected onto a line $i$. If $N$ is a point of the region having location vector $x_N$, then the assigned value from line $i$ will be $Z_i(\tau_{Ni})$ where $\tau_{Ni}$ is the projection of the vector $x_N$ onto line $i$ (see Figure 4.15). For each line, generate an independent realization using $C_1(\tau)$ as the covariance function. Generate $L$ lines such as $i$. Then at every point $N$ of the region, there are $L$ assigned values $Z_i(\tau_{Ni}) = Z_i(x_N^i u_i)$, where $i = 1, \ldots, L$, and $x_N^i u_i$ represents the inner product of the vector $x_N$ and the unit vector $u_i$. Finally, assign to the point $N$ the value $Z_S(x_N)$ given by:

$$Z_S(x_N) = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} Z_i(x_N^i u_i) \quad (4.7)$$

as the realization of the two- or three-dimensional random field.

If lines or planes are drawn perpendicularly to the line at the discrete ends of each discretized segment, a set of bands is defined (Figure 4.16). As the lines turn the bands defined above also turn. Thus, the method was given the name "Turning Bands Method" by Matheron (1973).

Figure 4.17 shows a conductivity field simulated by the TBM model which was developed by Mantoglou and Wilson (1981). The highest hydraulic conductivity region in general is located on the top of the map and an isolated area with higher hydraulic conductivity than its surrounding area is located to the right central region. The hydraulic
FIGURE 4.16 Definition of a Band on a Turning Bands Line
(from Mantoglou and Wilson, 1981)
FIGURE 4.17  Random Conductivity Field
30 ft x 30 ft domain
conductivity field was input to the MMOC method which was then simulated with the same set of parameters as in the grid-refinement convergence study for the purpose of a direction comparison. Concentration contours at 10 days and 20 days after injection were plotted in Figures 4.18 and 4.19. Figure 4.18 shows the plume is transported more rapidly in the upper areas with higher hydraulic conductivity during the first 10 days after injection. The plume pattern is skewed to the right before it reaches the pumping well, while the plume was symmetrically distributed along the diagonal connecting two wells in the case of uniform hydraulic conductivity field (Figure 4.9). A sharp left turn of the plume above the pumping well is seen in both Figure 4.18 and Figure 4.19, due to a higher hydraulic conductivity zone in that region.

A more interesting simulation was performed on a 1000 ft x 1000 ft domain with a more randomly distributed hydraulic conductivity field. Figure 4.20 shows the random hydraulic conductivity field in which the dense areas represent high hydraulic conductivity zones with contrasts of low zones as large as two orders of magnitude. The following parameters are used for this simulation:

\[ Q = 200 \text{ ft}^3/\text{day-ft} \]
\[ n = 0.3 \]
\[ \alpha_x = 10 \text{ ft} \]
\[ \alpha_y = 1 \text{ ft} \]
\[ n = 0.1 \]
FIGURE 4.18  Relative Concentration Contours
10 days after injection
FIGURE 4.19  Relative Concentration Contours
20 days after injection
FIGURE 4.20 Random Conductivity Field
in a 1000 ft x 1000 ft Domain
The injection well and the pumping well are placed at the coordinates (175 ft, 125 ft) and (875 ft, 125 ft), respectively. In Figure 4.21, the relatively higher hydraulic conductivity zones cause the front 240 days after injection to advance in a pattern commonly referred to as fingering. The front is transported more rapidly in the zones of higher hydraulic conductivity which is obvious from this figure. Figures 4.22 and 4.23 show the front at 520 days and 1000 days after injection, respectively. In these two figures, the low hydraulic conductivity area to the right of the pumping well apparently slows down the tracer movement before its arrival to the pumping well. An isolated "island" is left behind the main stream of the plume after 1000 days of injection in Figure 4.23.
FIGURE 4.21  Relative Concentration Contours
240 days after injection
(42 x 42 grid)
FIGURE 4.22  Relative Concentration Contours
520 days after injection
FIGURE 4.23  Relative Concentration Contours
1000 days after injection
CHAPTER FIVE

5.1 DISCUSSION

The MMOC method was compared with two analytical solutions, one with a single injection well and the other with an injection-pumping well pair. Excellent matches were demonstrated between the MMOC method and analytical solutions. The MMOC method was also compared with the USGS Solute Transport model on a 30 x 30 grid system and on a 60 x 60 grid system in a 30 ft x 30 ft domain. Much more accurate solutions were obtained from the MMOC method than the USGS Solute Transport model on both grid systems. In addition, the MMOC method was allowed to take as much as 14 times larger time steps than the USGS model to achieve similar resolutions. However, it is not presently clear which model requires less total CPU time to simulate an identical case. These two models were simulated on two different computers. The MMOC method will be loaded to the RICE main frame computer for a direct comparison in the near future.

One of the many advantages of the MMOC method over other numerical models is its flexibility to allow nonuniform grid systems, which has significant applications to groundwater contaminant transport. Away from wells, the groundwater seepage velocity does not vary rapidly in space and therefore relatively coarser grid intervals can be placed in
that region, while velocity travels much more rapidly near wells and the concentration front is very sharp and therefore fine grid intervals are required near wells. As with standard Galerkin finite element methods, the MMOC method requires fine enough grid intervals to resolve sharp concentration fronts. Through this nonuniform placement of grid intervals not only computing time is saved but also more accurate simulations are achieved.

A highly advective-dominated simulation with the Peclet number equal to 1000 proved the MMOC method was free of the numerical dispersion or oscillation problems which have plagued many other numerical methods in the past decades. The ability to simulate a highly advective-dominated problem has a potential linkage with the recent developed advection-diffusion concept to explain the scale-dependent dispersivity. For a perfectly stratified-layered aquifer system, the advection-diffusion concept treats the high permeability zone as a plug flow with infinite Peclet number. Therefore the MMOC method could be used as a profile model that simulates transport in high permeability layers, which is then linked with the diffusion equation for the low permeability layer's simulation. Through this linkage, the advection-diffusion concept can be tested in three-dimensional simulation versus two-dimensional simulation in Gillham et. al.'s paper (1984).
The ability to simulate random hydraulic conductivity fields provides another alternative to explain the scale-dependent dispersivity. Since the scale-dependent dispersion has been related to hydraulic conductivity through stochastic analyses in more recent research activities (Mercado, 1967; Schwartz, 1977; Gelhar et. al., 1979), the MMOC method, a simulator for the standard form of the advection-dispersion equation, combines with a random field simulator (Turning Bands or Monte Carlo) can be compared directly on an available field site with the stochastic models by Gelhar et. al. (1979). This comparison will not only test the conventional approach to the groundwater contaminant transport but also will test the validity of the stochastic equations in Gelhar et. al. (1979).

5.2 CONCLUSIONS

The MMOC method shows excellent potential application to a variety of groundwater contaminant transport problems. The following conclusions are drawn from this research:

1. MMOC has been tested against a known analytical solution to a single injection well for a special boundary condition (Figures 4.1 and 4.2). Good agreement between the MMOC method and the analytical solution was shown. The single injection analytical solution was shown by Wilson and Miller (1978) to accurately predict a contaminated plume in Long Island, N.Y.
2. MMOC has been compared with an analytical solution for an injection-pumping well pair which was developed by Grove and Beemem (1971). Excellent matches were demonstrated through comparisons with breakthrough curves at the pumping well (Figures 4.4 and 4.5).

3. MMOC and the USGS Solute Transport model have been compared with and analytical solution for an injection-pumping well pair. MMOC simulations agreed much more closely with the analytical solution than those of the USGS Solute Transport model (Figures 4.4 and 4.5). In addition, the MMOC method was allowed to take time steps 14 times as large as the USGS Solute Transport model for similar resolutions.

4. MMOC method has low core storage requirements due to an efficient preconditioned conjugate gradient solver for matrix operations.

5. MMOC has low numerical mass balance error (less than 2% in general).

6. Nonuniform placement of grids is allowed in the MMOC method. This flexibility not only saves computing time but also results in more accurate approximations.

7. MMOC method has been applied to highly advective-dominated flow fields with the Peclet number equal to 1000. Results showed this method has no numerical dispersions or oscillations problems.

8. MMOC method has been applied to random hydraulic conductivity fields that were simulated from the Turning Bands Method. Results showed that concentration fronts moved more rapidly in the zones of higher hydraulic conductivity and "fingers" developed in the plume. The ability to simulate random hydraulic conductivity fields potentially would provide another alternative to explain the scale-dependent dispersivity.
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APPENDIX I

PROGRAM ANALY
DIMENSION X(100), Y(100), C(100, 100)
1 , CC(100, 100), ICC(20000), X1(100), Y1(100)
NX=37
NY=29
NY1=2*NY-1
NX1=40
T=2000.
FM=214579.2
READ(5,5) Y(I), I=1, NY
READ(5,5) Y1(I), I=1, NY1
READ(5,5) X(I), I=1, NX
READ(5,5) X1(I), I=1, NX1
5 FORMAT(5F10.2)
PAI=3.14159265
PHI=0.35
V=1.5
ALPHX=69.9
ALPHY=14.0
DX=ALPHX*V
DY=ALPHY*V
B=2.0*ALPHX
DD 200 I=1, NX
IB=(I-1)*NY
DD 300 J=1, NY
RRSD=X(I)**2+ALPHX/ALPHY*(Y(J))**2.
RR=RRSD**0.5
VEL=RRSD/(4.*ALPHX*V**T)
RBETA=-(RR/B-2.*VEL)/(2.*VEL**0.5)
RBB=RR/B
WELLFN=(PAI/2./RBB)**0.5)*(EXP(-RBB))**ERFC(RBETA)
1 C
WELLFN=(PAI/2./RBB)**0.5)*(EXP(-RBB))
C 1 ((1.-1.)/(B.*RBB))**ERFC(RBETA)+(-RBETA/(4.*RBB*PAI**0.5))
1 C
#EXP(-RBETA**2.))
C(I,J)=FM*EXP(X(I)/B)/(4.*PAI*PHI*(DX*DY)**0.5)
1 #WELLFN
300 CONTINUE
PRINT 400, (C(I,J), J=1, NY)
400 FORMAT(1X, 5F10.3)
200 CONTINUE
DD 30 I=1, NX1
DD 30 J=1, NY1
30 CC(I,J)=0.
DD 40 I=1, NX
DD 40 J=1, NY
CC(I+3,J+NY-1)=C(I,J)
CC(I+3,NY-J+1)=C(I,J)
40 CONTINUE
DD 60 I=1, NX1
IB=(I-1)*NY1
DD 50 J=1, NY1
CC(I,J)=CC(I,J)/36.5/28.32
IF (CC(I,J)>0.1) ICC(I,J)=1.
ICC(IB+J)=CC(I,J)**1.0E+04
50 CONTINUE
WRITE(6, 1988) ICC(IB+J), J=1, NY1
60 CONTINUE
1988 FORMAT(1X, 15I5)
STOP
END
**APPENDIX II**

```plaintext
DIMENSION CON(20), T(20)
PORO=0.3
DH=0.7
PAI=3.14159265
PINC=PAI/180.
A=3.
Q=1.5
T(1)=1.
DO 10 I=2,20
   T(I)=T(I-1)*1.
10 DO 30 J=1,20
   CON(J)=4.*
   ALPHA=0.
   DO 20 Y=1,150
      ALPHA=ALPHA+PINC
      SINA=SIN(ALPHA)
      C PRINT*, SINA
      TL=2.*ALPHA/SINA
      PLT=4.*PAI?PORO*4.*A*(ALPHA*COS(2*PI*SINA)-4.)/(Q*SIN(ALPHA)
      +SIN(ALPHA))
      PLT=ABS(PLT)
      TP=T(3)/PLT
      PEC=TL/(1.*DM)
      RATIO=PEC/TP
      C PRIN*, RATIO
      ARG0=SRT(PEC/TP)*(1.-TP)
      IF(ARG0.LT.0.)GO TO 40
      TMP=0.5*ERFC(ARG0)
      GO TO 50
      40 TMP=0.5*(1.*ERF(-ARG0))
      50 TMP2=SQRF(4.*PEC/TP/PAI)*(3.+2.*PEC*(1.+TP))
      ARG1=PEC*(1.-TP)*(1.-TP)/TP
      IF(ARG1.GE.195.)ARG1=195.
      C PRINT*, ARG1
      TMP3=EXP(-ARG1)
      TMP4=0.5*2.*PEC*(3.+4.*TP)+4.*PEC*PEC*(1.+TP)*(1.+TP)
      ARG2=4.*PEC
      IF(ARG2.GE.195.)ARG2=195.
      C PRINT*, ARG2
      TMP5=EXP(ARG2)*ERFC(SRT(PEC/TP)*(1.+TP))
      FINAL=TMP1+TMP2+TMP3+TMP4+TMP5
      IF(FINAL.LE.0.)FINAL=0.
      CON(J)=CON(J)+FINAL
      20 CONTINUE
      30 CONTINUE
      DO 70 I=1,20
         CON(J)=CON(J)/180.
         WRITE(6,50)CON(J), J=1,20
      50 FORMAT(6,5F13.7)
      STOP
      END
```
APPENDIX III

Start

Input data

Compute radial concentration at injection wells according to the 1-D radial equation (Eq. 3.21)

Least-square projection of the radial concentration onto the tensor-product space. The L2 projection matrix is calculated based on the continuous bilinear basis function and the preconditioned conjugate gradient iteration is used to solve for projected concentration.

Compute the source and sink terms of Eq. 3.37

Compute time-independent constant for concentration calculation. Calculate the necessary polynomial roots and the corresponding weight factors and set up numerical integration for all matrix terms corresponding to the left hand side of Eq. 3.18.
Compute time-dependent constants of one time step for the concentration calculation. Lobatto points and Gauss points in the concentration grid system are located in the corresponding hydraulic grid system.

Compute entries of the matrix and the right hand side of Eq. 3.37 which is the final form of the mixed finite element formulation.

Compute block centered finite difference matrix as a preconditioner for Eq. 3.37.

Use the preconditioned conjugate gradient method to solve Eq. 3.37 to obtain Darcy velocity and hydraulic head simultaneously.
Loop through concentration time step

Compute "average" velocity $V^*$ at each time step and at all concentration quadrature points backward in time, in segments. Each segment covers an adaptively selected length of time -- micro-time step.

Set up matrix and right hand side for one concentration time step (Eq. 3.18). The matrix is formed by piecing up rectangles over the concentration mesh. Each rectangle includes diffusion-dispersion and capacity terms. The source term is included in the injection rectangles.

Use the preconditioned conjugate gradient method to compute new concentration. The right hand side calculates the old concentration (previous time step) at each characteristic point from a backward tracing of the "average" velocity.

Computer material balance statistics

End