Numerical Simulation of Saturated Flow with Fractal Analysis of the Hydraulic Conductivity Distribution

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Numerical Simulation of Saturated Flow with Fractal Analysis of the Hydraulic Conductivity Distribution

by

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Introduction

The purpose of this report is to investigate the behavior of a nonreactive contaminant in a perfectly stratified aquifer under uniform, steady-state flow. The design and the implementation of a solute transport model which characterizes the heterogeneities of the aquifer properties in a stochastic framework is reviewed. The model closely examines the advection and dispersion of the plume. The advection is the process by which the plume is transported in the aquifer by the bulk average motion of the groundwater whereas the dispersion refers to the spreading of the plume about its mean displacement position. The relationship between the fractally distributed hydraulic conductivity and the extent of spreading is the focus of investigation.

The heterogeneous hydraulic conductivity field is generated by a one-dimensional fractal generator as discussed by Meija (1984)[12]. The flow simulations are based on the mixed finite element method and the finite difference method is employed to solve the advection-dispersion (transport) equation. The simulator SIM2D2P uses the IMPES (IMPlicit Pressure Explicit Saturation) algorithm which approximates
the pressure and velocity explicitly at the next time step and explicitly updates the saturation with the results.

The motivation for these simulations stems from a need to study the contaminant dispersion in heterogeneous porous media. Although there are numerous simulations that purport to achieve same objectives, this particular method of simulation is different in two very important ways. First, the hydraulic conductivity field is assumed to be fractal in nature. Second, an accurate numerical scheme has been employed to approximate the velocity. In this report, it will be examined how these differences affect the behavior of the contaminant dispersion. The results of the simulations are compared to the analytic results developed by Kemblowski [9].

In the first chapter, the background statistics is presented. In the second chapter, the computational scheme is described and some analysis is performed on the transport equation. The numerical results are presented in the third chapter. The text is followed by tables and figures that present the numerical results.
Chapter 1

Groundwater Statistics

1.1 Stochastic Analysis of Plume Dispersion

The natural heterogeneities of the aquifer materials in a porous medium provide sufficient motivation for using a stochastic approach to describe the groundwater problems. Although a deterministic approach that represents the actual heterogeneities would be preferred, the limit in the computational and economic resources render such an attempt neither pragmatic nor feasible. In addition, a deterministic transport model merely interpolates a discrete number of points of a aquifer parameter and consequently, there will always remain scales of heterogeneities that are not modeled in the process. A stochastic model, on the other hand, provides invaluable insights without exhausting resources at hand. In recent literature, spectral methods have
been actively employed to represent the variability of hydraulic conductivity where the conductivity is a stochastic process [1, 4].

In a stochastic framework, the hydraulic parameters are treated as random quantities or processes. One such hydraulic parameter that is crucial in the analysis of the contaminant plume transport in groundwater is the hydraulic conductivity, $K$. In simple terms, the hydraulic conductivity can be considered a measure of how easily the fluid flows through the porous medium. A medium has a unit hydraulic conductivity if it will transmit, in unit time, a unit volume of groundwater through a cross-section of unit area. The hydraulic conductivity which is measured in terms of distance per time is an intrinsic property of the medium and is independent of the fluid properties.

In order to understand the statistical properties, we will use to describe the hydraulic conductivity as a random process, it is necessary to present a few general but relevant statistical concepts.

### 1.2 Background Statistics for Random Process, $X$

A convenient way to obtain the probabilities is to use a probability distribution. Initially consider the hydraulic conductivity as a random process, say $X_z$ where $z$ is the location variable. Any random variable, $X_z \in X$, has a density function denoted by $B_z(x)$ or $B(x)$. 
The integral \( \int_a^b B(x) \, dx \) is the probability that the random variable, \( X \), will fall in the interval \((a,b)\). In traditional approaches to groundwater statistics, the hydraulic conductivity is considered to be lognormally distributed; the probability density for a lognormal distribution is

\[
B(x) = \frac{1}{\sqrt{2\pi \sigma x}} \exp\left[-\frac{1}{2\sigma^2}(\ln x - \mu)^2\right], \quad x > 0, \quad -\infty < \mu < \infty, \quad \sigma > 0
\] (1.1)

An alternative approach that is steadily gaining popularity in the literature is to assume that the distribution of the hydraulic conductivity is fractal in nature [6, 8]. In later sections, fractals will be examined more closely.

Moments are quantities that are often used to describe the behavior of hydraulic conductivity. The first moment is the usual mean value, which is given by

\[
\mu_X = E[X] = \int_{-\infty}^{\infty} x B(x) \, dx
\] (1.2)

and is read as the "expected value of \( X \)." The variance of \( X \) is given by the central second moment and is defined as

\[
E[(X - E[X])^2] = \int_{-\infty}^{\infty} (x - E[X])^2 B(x) \, dx
\] (1.3)

The central second moment or commonly known as the variance of the random variable, \( X \), measures the amount of spread of \( X \) values from its mean value, \( E[X] \). As will be seen more clearly in later sections, the dispersivity of the contaminant plume is proportional to the variance of the hydraulic conductivity.
The probability density of two variables is called the joint probability density. If there exists a function, \( B(x, y) \) for all \( x \in X \) and \( y \in Y \), then we say \( X \) and \( Y \) are jointly continuous. The probability that \((X, Y)\) is in the small neighborhood of \((x, y)\) is proportional to \( B(x, y) \).

The covariance of any two random variables, \( X \) and \( Y \) denoted by \( \text{Cov}(X, Y) \) is defined by:

\[
\text{Cov}(X, Y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (x - E[X])(y - E[Y])B(x, y)\,dx\,dy \tag{1.4}
\]

where

\[ E[X] = \text{expected value of } X \]

and

\[ E[Y] = \text{expected value of } Y \]

The covariance measures the relationship between the two random variables and indicates the extent of asymmetry of the joint distribution. If \( B(x, y) = B(-x, y) \), then the \( \text{cov}(X, Y) = 0 \). In turn, if \( \text{cov}(X, Y) = 0 \), then we say that the random variables, \( X \) and \( Y \), are uncorrelated or orthogonal.

To describe the hydraulic conductivity as a random process, the values of \( X \) at different spatial points needs to be considered. The covariance between the values of \( X \) at two different spatial values is called the autocovariance. If the random field is homogeneous, the autocovariance function will depend on the relative position of
the two spatial locations and becomes a function of $l$. Physically, this implies that
the hydraulic conductivity at any given spatial point of an aquifer can be related to
other spatial points. The distance between the two spatial points where the hydraulic
conductivity is the same can be thought of as being the correlation length or a lag
vector. In this specific case, the process $X$ is called stationary ($E[X_z] = E[X_{z+l}]$) and
the autocovariance function is defined as

$$C_x(l) = E[X_{z+l}X_z] - E^2[X]$$  \hspace{1cm} (1.5)

where $l$ = lag vector.

1.3 Spectral Analysis of the Hydraulic Conductivity

Much of the statistical analysis of the hydraulic conductivity as a random process
can be facilitated by the introduction of the function known as the spectral density.
Many of the statistical properties that we discussed can be derived and elaborated
on in the "frequency domain."

The variance properties of frequency can be considered through spectral analysis
in which the rate at which the series oscillate is defined in terms of its frequency, $\omega_k$. 

The random variable, $X_z \in \mathbf{X}$ can be decomposed as

$$X_z = \mu_X + \sum_{k=-K}^{K} X_{zk}$$

(1.6)

and

$$X_{zk} = C_k \cos(\omega_k z + \Phi_k)$$

(1.7)

where

$$\mu_X = E[X_z]$$

$$\omega_k = \pm[\Delta \omega(2k - 1)/2]$$

$$C_k = \text{random amplitudes}$$

$$\Phi_k = \text{phase angles, uniformly distributed on } (0, 2\pi)$$

Here, $C_k$'s are considered mutually uncorrelated. A simple computation shows that the random function $X_{zk}$ has a mean zero and variance

$$\sigma^2_k = E[X_{zk}] = E[C_k^2] E[\cos^2(\omega_k z + \Phi_k)] = \frac{1}{2} E[C_k^2]$$

(1.8)

Hence, the variance of random process, $X_z$ is

$$\sigma^2 = \sum_{k=-K}^{K} \frac{1}{2} E[C_k^2]$$

(1.9)

The spectral mass function is defined as

$$S(\omega_k) \Delta \omega = \frac{1}{2} E[C_k^2] = \sum_{k=-K}^{K} \sigma^2_k$$

(1.10)
which expresses the total variance of the series $X_z$ as the sum of variance contributions at all the frequencies.

By letting $\Delta \omega \to 0$ and $K \to \infty$, the variance $X_z$, $\sigma^2$ can be rewritten as

$$\sigma^2 = \sum_{k=-K}^{K} S(\omega_k) \Delta \omega \to \int_{-\infty}^{\infty} S(\omega) d\omega \quad (1.11)$$

where $S(\omega)$ is the spectral density of $X_z$. The spectral density function is not a density function of a random variable but it is what statistician call the power spectrum.

For the stationary process, the spectral density function can also be found by taking the Fourier transform of the covariance function, $C_x(l)$ as follows [3]

$$S_X(f) = \frac{1}{2\pi^3} \int_{-\infty}^{\infty} \exp(-i\omega l)C_x(l)dl \quad (1.12)$$

where

$l = \text{lag vector}$

and

$f = \text{wave number}$

### 1.4 Fractals

The classical stochastic approach assumes that the heterogeneities are relatively small compared to the overall scale of observation. It also assumes that the hydraulic conductivity is a stationary process with bounded fluctuation variance. However,
a detailed study of various sites where the field tests on hydraulic conductivity are conducted indicates that this assumption is questionable [2]. It appears that the subsurface materials possess long-range correlations. These properties can be modeled with fractals which are self-similar models of objects with theoretically infinite correlation lengths.

Mandelbrot's fractal geometry provides a mathematical framework for describing complex natural phenomena found in nature. Fractals are characterized by self-similarity by which an object consists of N copies of itself. Self-similarity can be perfect as in Koch snow flake or statistical as objects found in nature. The shapes of nature such as clouds, mountains, and coastlines have construction that can not easily described by Euclidean notion of geometry. The perceptual difference, according to Mandelbrot, among different natural phenomena are due to differences in the value of a parameter, D or fractal dimension [11].

The fractal dimension, D, which corresponds to our intuitive notion of dimension is not necessarily an integer. Consider a set, S, of points, \(x = (x_1, \ldots, x_E)\) in Euclidean space of dimension, \(E\). Under the similarity transform, using a scaling factor, \(0 < r < 1\), the set \(S\) becomes \(rS\) where \(rx = (rx_1, \ldots, rx_E)\). A bounded set, \(S\), is self-similar if \(S\) is a union of N disjoint subsets, all of each is congruent to \(rS\). Then the fractal dimension is defined as

\[
1 = N r^D \tag{1.13}
\]
1.5 Application of Fractals to Describe Hydraulic Conductivity

The traditional stochastic analysis of groundwater assumes that the variogram or variance of increments is bounded by the aquifer property’s variance [7].

\[
\lim_{l \to 0} \gamma(l) = 0.5E[(X_{x+l} - X_x)^2] = \sigma_x^2
\]  

(1.15)

However, since a fractal distribution has correlation over all scales, the variogram is not bounded and is described by the power law.

\[
\gamma(l) = \gamma_1 l^{2H}
\]  

(1.16)

where

\[ \gamma_1 = \text{value of the variogram at } l = 1 \]

and

\[ H = \text{fractal codimension (E-D)} \]

The correlations over all scales allow the variation of any scale, \( rl \), to be written in terms of the variation over a chosen scale by the equation

\[
\gamma(rl) = \gamma(l) r^{2H}
\]  

(1.17)
This results shows that the variance of any scale can be found by estimating a variance of any other scale. This, in turn, implies that the variance of $K$ is scale dependent. Combining the equations for the autocorrelation and the variogram yields another expression for the variogram

$$\gamma_\mathbf{X}(l) = E[X_z^2] - E^2[X_z] - C_\mathbf{X}(l)$$  \hspace{1cm} \text{(1.18)}

Using this expression for the variogram and the Wiener-Khintchine [6] theorem, the autocovariance function, $C_\mathbf{X}(l)$ can be expressed as

$$C_\mathbf{X} = \int_0^\infty S_x(f)\cos(2\pi fl)df$$  \hspace{1cm} \text{(1.19)}

where $S_f$ = spectral density of $X_z$

It can be shown that for a fractal distribution, the spectral density of a variable, $X_z$, follows another form of power law [6]

$$S_\mathbf{X}(f) = S_1 f^{-\beta}$$  \hspace{1cm} \text{(1.20)}

where

$S_1$ = spectral density at $f = 1$(or intrinsic variance)

and

$\beta$ = fractal codimension ($=2H+1$)

Many of the analyses using the fractal approach show that the fractal dimension is between 1.75 and 2 for the vertical hydraulic conductivity distribution [8]. A high
magnitude of the vertical fractal dimension indicates highly chaotic nature of the distribution. On the other hand, the horizontal fractal dimension is estimated to be significantly less (D=1.475 for the Berino Site [8]). From these results, it can be concluded that the horizontal hydraulic conductivity distribution exhibits increments that are correlated over a finite distances whereas the vertical distribution displays long range correlation. The chaotic nature of the hydraulic conductivity distribution will induce a highly irregular plume surface which will in turn reduce the dispersive effects.
Chapter 2

Numerical Experiment

2.1 Numerical Method

The numerical simulation of a perfectly stratified porous medium under steady-state uniform flow is performed as a case study of the movement of a contaminant through a porous medium. The primary aim is to numerically solve the governing partial differential equations for contaminant mass and compute the mass moments to analyze the spreading of the plume. Specifically, the simulation sheds light on the time and spatial effects of the flow field as the tracer plume expands over time. In chapter 3, the numerically computed macrodispersivity from the simulation will be compared to theoretical predictions based on the stochastic analysis. In this chapter, the governing equations and the numerical method will be presented.
2.2 Governing Equations

The steady saturated flow equation in a heterogeneous porous medium is given by

$$\nabla \cdot K(x) \nabla h = 0, \ x \in \Omega, \ h_o > h_1$$ \hspace{1cm} (2.1)

where

$$h_o = \text{fixed head on the inflow boundary}$$

$$h_1 = \text{fixed head on the outflow boundary}$$

$$h = \text{hydraulic head and}$$

$$K(x) = \text{hydraulic conductivity}$$

$$\Omega = [0,1] \times [0,1]$$

The trivial solution for the partial differential equation is \( h = 0 \). The typical boundary conditions are fixed heads on two opposite sides and no flux on the remaining boundaries of a square domain. The potential form of the Darcy’s equation for average pore water velocity is

$$v_i = -\frac{K}{n} \frac{\partial h}{\partial x_i}$$ \hspace{1cm} (2.2)

where \( n = \text{porosity} \)

The governing equation that describes the motion of the conservative solute in two-dimensional porous medium is given by

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x} \left( UC \right) = \frac{\partial}{\partial x} \left( D_L \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial z} \left( D_T \frac{\partial C}{\partial z} \right)$$ \hspace{1cm} (2.3)
where

\[ C = \text{concentration of the solute} \]

\[ U = \text{Darcy flux} \]

\[ D_L = \text{longitudinal dispersion tensor} \]

\[ D_T = \text{transversal dispersion tensor} \]

\[ x = \text{domain in the flow direction} \]

\[ z = \text{domain perpendicular to the flow direction} \]

\[ t = \text{time} \]

A mixed finite element method is used to implicitly solve the system of partial differentiation equations for flow (that is, solve for \( h \) and \( v \)) coupled with an explicit finite difference method for the concentration. This IMPES (IMplicit Pressure Explicit Saturation) simulator which originally has its application in petroleum-related problems is adopted as the main algorithm for solving the governing equations.

### 2.3 Dimensional Analysis of the Governing Equation

Scaling is an important task in the analysis of the numerical results obtained from the numerical experimentation. There are two major considerations that need to be referred to before appropriate parameters and dimensions are selected for the given
problem. First involves the compatibility of units and dimensions to the field data. The variables such as size of the domain, total amount of transport time, and so forth need to have some foundation on the actual field-based data.

The second consideration involves the compatibility of the chosen dimensions with the machine storage at hand. For instance, if the plume takes approximately 500 days to achieve the asymptotic behavior as it propagates at the speed of 2~5 meters a day, the CFL condition dictates that the length of the domain in the flow direction be at least 125 cells. This raises the question of feasibility particularly when the resources at hand are limited. One scheme that allows flexibility in scaling while simultaneously satisfy both these considerations involves the nondimensionalization of the problem. The motivation behind such endeavor is clear as the above considerations indicate. Table A.1 presents the corresponding units for each parameter that appears in the equation 3. The next step of the analysis involves the selection of characteristic scales and rewriting the governing equation in a dimensionless form. Nondimensionalization will be performed on the transport equation. If \( p \) is the variable, let \( p_c \) be its intrinsic scale, appropriate to the given model. Then a new dimensionless variable \( \bar{p} \) can be defined as

\[
\bar{p} = \frac{p}{p_c}
\]  

(2.4)

The advection-dispersion equation for nonreactive dissolved constituents consists of the convective expression on the left hand side and of the diffusive expressive on
the right hand side. The dispersion tensor as implemented in the SIM2P2D code is

$$\nabla D \nabla C = \xi \nabla \cdot \left[ \frac{\omega_L}{||U||} \begin{pmatrix} U_x^2 & U_x U_z \\ U_z U_x & U_z^2 \end{pmatrix} + \frac{\omega_T}{||U||} \begin{pmatrix} U_z^2 & -U_x U_z \\ -U_z U_x & U_x^2 \end{pmatrix} \right] \nabla C \quad (2.5)$$

where

$$w_L = D_L x_c$$

$$w_T = D_T x_c$$

$$U = \text{Darcy velocity}$$

$$\xi = \text{input parameter that determines the magnitude of}$$

the diffusion coefficient

$$x_c = \text{characteristic domain length}$$

$$||U|| = \text{magnitude of flux}$$

The parameters, $D_L$ and $D_T$, are employed to control the relative differences in the transverse and longitudinal dispersive effects. If isotropy is assumed, the transverse and longitudinal dispersion can be assumed equal and therefore, $D_L$ and $D_T$ are the same and assumed to be equal to one.

In the two-dimensional representation of the perfectly stratified aquifer under steady-state, uniform flow several assumptions can be made to simplify the diffusive side of the equation.

An isotropic scenario yields equality between $w_L$ and $w_T$. Furthermore, since the water flows from left to right in the two-dimensional domain with no flux conditions
on the boundaries that are transverse to the flow, the velocity in the $z$ direction, $v_z$, equals zero. Combined, this yields

$$\nabla D \nabla C = 2(\omega_L)(\xi)[\frac{\partial}{\partial x} \|U\| \frac{\partial C}{\partial x} + \frac{\partial}{\partial z} \|U\| \frac{\partial C}{\partial z}]$$  \hspace{1cm} (2.6)$$

Introduction of the nondimensional variables to the resulting advection-dispersion equation and the rearrangement of the characteristic scales yields the following nondimensional formulation of the equation.

$$\frac{\partial \bar{C}}{\partial \tilde{t}} + \alpha \frac{\partial}{\partial \tilde{x}} (\bar{U} \bar{C}) = \beta (\frac{\partial}{\partial \tilde{x}} \bar{U} \frac{\partial \bar{C}}{\partial \tilde{x}} + \gamma \bar{U} \frac{\partial \bar{C}}{\partial \tilde{z}})$$ \hspace{1cm} (2.7)$$

$$\gamma = \frac{x_c^2}{z_c^2}$$ \hspace{1cm} (2.8)$$

$$\alpha = \frac{u_c t_c}{x_c}$$ \hspace{1cm} (2.9)$$

$$\beta = \frac{2\omega_L(\xi) u_c t_c}{x_c^2}$$ \hspace{1cm} (2.10)$$

The parameters $\alpha$ and $\beta$ measure the convective and dispersive effects of the flow on the plume, respectively. The ratio of $\alpha$ and $\beta$ which is more commonly known as the Peclet number measures the relative magnitude of diffusion to convection. Cancellation of the like terms leads to the following simpler version of the ratio.

$$\frac{\alpha}{\beta} = \frac{1}{2\xi}$$ \hspace{1cm} (2.11)$$
When simulating flow and contaminant transport in groundwater, the modeling scale must be chosen that is consistent with the contaminant travel distances. These travel distances depend on the heterogeneities of the geological properties. The effect of diffusion to convection must be balanced to satisfy the constraints as posed by the heterogeneities and modeling scale. Therefore, the major consideration concerns the balanced effect of diffusion to convection. The dimensional analysis of the transport equation indicates the desired effect can be implemented by varying $\xi$, the input parameter. If $\xi$ is too large, the dispersive process dominates, the pore level effects render the effects of aquifer negligible. On the other hand, if $\xi$ is too small, the convective process dominates and any meaningful statistical analysis becomes difficult particularly when the domain is small and/or the pore water velocity is high.

2.4 Truncation Error Analysis

The numerical scheme does not necessarily provide an accurate approximation to the true solution. The convergence of a finite difference scheme can be investigated by calculating the truncation error which measures the error that results from replacing the derivatives of the equation by the difference expressions. The governing partial differential equation (eq.3) can be represented as

$$\delta(u,c) = 0, \ (x,z) \in \Omega$$  \hspace{1cm} (2.12)
where δ is the differential operator. Another operator, δΔ can be defined to represent the difference equation.

\[
\delta_{\Delta}(U, C) = 0, (x, z) \in \Omega_\Delta
\]  

(2.13)

The truncation error, τ, is defined to be the difference between the partial differential equation and the difference approximation.

\[
\tau = \delta(u, c) - \delta_{\Delta}(U, C), (x, z) \in \Omega_\Delta
\]  

(2.14)

It can be found that the truncation error that accompanies the advection-dispersion equation is

\[
\tau_{i,j,n} = -\frac{\Delta t^2}{2}(C_{tt})_{i,j}^n + \frac{\Delta x}{2}\alpha U_j(C_{xx})_{i,j}^n +
\]

\[
\beta\gamma\frac{\Delta z^2}{4}(C_{zz})_{i,j}^n(U_{zz})_{i,j}^n + \beta\gamma((C_z)_{i,j}^n(U_{zzz})_{i,j}^n +
\]

\[
(U_{zzz})_{i,j}^n \frac{\Delta z^2}{6} + (C_{zz})_{i,j}^n(U_{zzz})_{i,j}^n \frac{\Delta z^4}{36} = O(\Delta x) + O(\Delta z) + O(\Delta t^2)
\]

(2.15)

Therefore, the truncation error is second order in Δt, and first order in Δx and Δz.

Furthermore, τ tends to zero as Δx → 0, Δt → 0, and Δz → 0.
Chapter 3

Numerical Results

3.1 Description of the Problem

This chapter describes the numerical investigation of macrodispersivity and analysis of the numerical results. The scenario under consideration is a simple one; a nonreactive solute is transported through a perfectly stratified aquifer. It is assumed that the groundwater flows horizontally from left to right and that the vertical distribution of the hydraulic conductivity, \( K \), is fractal in nature.

The numerical scheme that is described in the previous chapter is employed to solve the governing partial differential equation. The vertical distribution of \( K \) is generated using the spectral method where it is assumed that \( K \) is a fractal object and therefore, follows the power law (eq.1.21). Meija’s scheme is adopted to generated
the actual distribution of $K$ [12]. The generation is performed by the equation

$$X(z) = 2 \sum_{k=1}^{M} (S_0 f_k^{-\beta} \Delta f^\frac{1}{2} \cos(f_k' z + \Phi_k))$$  \hspace{1cm} (3.1)$$

where $\Omega =$ transport domain

$$\Delta f = \Omega / M , \text{discretization frequency}$$

$$f_k = (k - \frac{1}{2}) \Delta f$$

$M =$ number of discrete frequencies in the approximation

$$\Phi_k =$ independent random angles, uniformly distributed in $[0, 2\pi]$ 

$$\beta =$ fractal codimension ($=5-2D$, where $D =$ fractal dimension)

$S_0 =$ intrinsic variance

The frequency, $\delta f$ is uniformly distributed in $[-\frac{1}{2} \Delta f', \frac{1}{2} \Delta f']$ where $\Delta f' \ll \Delta f$.

Uniform deviates which lie within a specified interval $[a,b]$ are produced by initially generating random deviates uniformly distributed on the interval $[0,1]$ and then translating them by the formula

$$Y_1 = (b - a) X_1 + a$$  \hspace{1cm} (3.2)$$

where $Y_1 =$ random deviate $\sim U[a,b]$

$$X_1 =$ random deviate $\sim U[0,1]$$

The variance of process $X$ depends on the spectral density value at $f=1$ which is also known as the intrinsic variance of process $X$. However, the process $X$ can be rescaled
to obtain a process \( K \) that has a specified mean \( \bar{K} \), and variance, \( \sigma_k^2 \) by using the formula

\[
K = \bar{K} + \sigma_k (X - \bar{X})/\sigma_x
\]  

(3.3)

where

\[
\sigma_x = \text{standard deviation of process } X
\]

and

\[
\bar{X} = \text{average value for process } X
\]

The domain chosen for the simulation is a square \([0,1] \times [0,1] \) region. The conservative, nonreactive tracer plume is released into the aquifer, initially void of any solute from a source that is midway along the left (inflow) boundary of the square domain. The plume thickness corresponds to the ten percent of the boundary. (See Figure B.1.)

The initial concentration of the plume is normalized so that the highest concentration corresponds to the centroid of the plume. Figure B.1 presents the concentration contour plot at the initial time step.

As the plume moves along a nearly linear trajectory, its shape and internal structure becomes modified as it encounters heterogeneities of the medium. Figure B.2 presents the typical concentration contour plot at the later stage of the plume transport. Examination of the plot indicates that the concentration distribution is skewed and the plume has dispersed to cover wider region of the flow domain.
3.2 Input Parameters

The major parameters that are considered for the simulation are fractal dimension, D, variance of K over the plume thickness, and the diffusion coefficient, $\xi$, (which is used as the approximation for the pore level transverse dispersivity, $\alpha_T$). The pore level transverse and longitudinal dispersivities are set to be equal to produce an isotropic hydraulic conductivity field.

In the first experiment, it is attempted to isolate the effect of the variance of K over the plume thickness, $L_o$, and the fractal dimension, D, by holding $\alpha_T$ constant at 0.00008904. Three different fractal dimensions (1.1, 1.5, and 1.9) are chosen for the simulation. These input parameters and a list of runs are given in table A.1 and table A.2, respectively.

To allow for the comparison between the numerically computed macrodispersivity and the theoretical macrodispersivity, it is necessary to compute the variance of K over the plume thickness, $L_o$. Three values for the variances of K are chosen: 100.0, 625.0, and 900.0. Since the variance of K over the whole domain is needed as an input parameter for the simulation, the following scheme is used to manually compute its value. This method is adopted because there is no explicit method for computing the intrinsic variance, which is an inherent parameter of the medium. If the plume thickness equals the length of the inflow boundary and the domain is a unit square...
the spectral density at $f=1$ (or the intrinsic variance) can be computed as follows

\[ S_0 = (\beta - 1)\sigma^2 \]  

(3.4)

where

- $S_0 =$ intrinsic variance
- $f =$ wave number
- $\beta =$ fractal codimension
  - $= 5 - 2D$, where $D$ is the fractal dimension
- $\sigma^2 =$ variance of $K$ over the domain

From this computed value of $S_0$, the variance of $K$ over the plume thickness, $L_0$, is estimated as follows

\[ \sigma_0^2 = \sigma^2(L_0) = \frac{S_0L_0^{\beta-1}}{\beta - 1} \]  

(3.5)

Combining equations 3.4 and 3.5 yields

\[ \sigma^2 = \frac{\sigma_0^2}{L_0^{\beta-1}} \]  

(3.6)

where $\sigma^2 =$ variance of $K$ over the whole domain. The computed values of $\sigma^2$ are listed in table A.3.
3.3 Computation of Asymptotic Macrodispersivity, $A_\infty$

The relationship for the asymptotic macrodispersivity, $A_\infty$, is as follows [9]

\[ A_\infty = \frac{2\sigma_y^2 L_0^2 (4 - 2D)}{\alpha_T \bar{K}^2 (6 - 2D)} \]  \hspace{1cm} (3.7)

where

\[ D = \text{fractal dimension} \]
\[ \bar{K} = \text{hydraulic conductivity over the plume thickness}, L_0 \]
\[ \alpha_T = \text{pore level transversal dispersivity} \]

In order to obtain a more accurate value of $\alpha_T$, the effect of numerical dispersion is considered. Instead of using the initial input value for local transverse dispersion coefficient (which is 0.00008904), a numerical experiment on a homogeneous medium where the value of $K$ is identically equal to 500 is performed. The conservative tracer is released and the numerical macrodispersivity is computed. This computed value is substituted for the pore level transversal dispersivity in equation. The computed values of asymptotic macrodispersivity, $A_\infty$, for each case run are listed in table A.4.
3.4 Computation of Numerical Macrodispersivity, $A_N$

The second moment measures the spread of the concentration distribution about the center of the mass of the plume, and therefore, the spreading of the plume along the longitudinal and transversal axes of the plume. The second moments are computed by the formulas

\[ \sigma_L^2 = \frac{\int_{[0,1]^2} C(x,y,t)(x-x_c)^2 dx dy}{M} \]  
\[ \sigma_T^2 = \frac{\int_{[0,1]^2} C(x,y,t)(y-y_c)^2 dx dy}{M} \]

where

- $C(x,y,t)$ = concentration
- $(x_c,y_c)$ = center of the mass coordinates
- $\sigma_L^2$ = second moment along the longitudinal axis
- $\sigma_T^2$ = second moment along the transversal axis
- $M$ = total mass

The second moment of particular interest is that of the longitudinal direction. The plots of the second moments, $\sigma_L^2$, are obtained for each case. Figure B.3 shows longitudinal second moment plots for $D=1.5$ and var($K$)=100.0, 400.0, and
900.0. All second moment curves follow a similar trend. The plots display a short-lived nonlinearity and then becomes linear in moderately early stage of the plume transport. This indicates that the plume reaches asymptotic behavior very early in its evolution.

A simple linear regression on the linear portion of the curve is employed to estimate its slope, \( \frac{d\sigma^2}{dt} \). This, in turn, is used to compute the dispersion coefficient

\[
D_L = \frac{1}{2} \frac{d\sigma^2}{dt}
\]  

(3.10)

The numerical macrodispersivity, \( A_N \), is computed by the equation

\[
A_N = \frac{D_L S_f}{V}
\]  

(3.11)

where

\( V \) = average pore water velocity and

\( S_f \) = scaling factor = 159.01393

Table A.5 presents the computed values of \( A_N \).

### 3.5 Analysis of the Results

An analysis of the obtained numerical results indicate a strong scale-dependence. As variance of \( K \) over \( L_o \) increases, the numerical macrodispersivity, \( A_N \), increases. The increase is pronounced for smaller fractal dimension (\( D=1.1 \)) than in larger fractal dimensions (\( D=1.5 \) or \( D=1.9 \)). Figure B.4 depicts the described behavior.
Figure B.5 shows the dependence of $A_N$ on the fractal dimension. It is clearly seen that the asymptotic macrodispersivity is a function of fractal dimension. As fractal dimension, $D$, increases, $A_N$ decreases. The finding coincides with the earlier finding that the larger fractal dimension induces more mixing between the layers, and therefore, less spreading in the longitudinal direction [9].

3.6 Comparison of $A_N$ to $A_\infty$

The values of $A_N$ and $A_\infty$ are compared in table A.4. Although there are discrepancies in the actual figures, the qualitative behavior of $A_N$ and $A_\infty$ coincide. Both show scale dependence and both are inversely proportional to the fractal dimension. However, there are two major discrepancies between $A_N$ and $A_\infty$ worth investigation. One is the effect of fractal dimension, $D$, on $A_N$. The values of $A_N$ experience sharp increase as $D$ is increased from 1.1 to 1.5, particularly in cases where the variances of $K$ are relatively large. The corresponding values of $A_\infty$ do not reflect the comparable magnitude in the increase. Another discrepancy is the minimal effect of variance of $K$ on $A_N$ for $D=1.9$. For $D=1.9$, although $A_N$ increases as the variance of $K$ increases, the increase remains very slight. From these findings, it can be deduced that the numerical simulation is more sensitive to the changes in the fractal dimensions (particularly for larger variances of $K$) than what is shown analytically. In addition, it appears that for large fractal dimension, the variance of $K$ does not influence the nu-
numerical macrodispersivity as it is expected analytically. Discrepancies for high fractal dimension can be explained by the highly chaotic nature that is associated with such dimensions. References indicate that larger fractal dimension induces behavior that is difficult to predict [8].
Conclusion

In this section, the highlights and findings of the report are recapitulated and additional avenues for further research are examined. The primary objective of the report is to investigate the spreading of the non-reactive contaminant in the perfectly stratified aquifer that is characterized by a fractally distributed hydraulic conductivity field. Unlike the conventional stochastic models, it is assumed that the correlation length of $K$ is theoretically infinite whereas the plume thickness is finite. The findings show that the spreading of the plume as measured by the second moment is dependent on the fractal dimension, $D$, and the plume thickness, $L_0$. Larger fractal dimensions indicate that the surface of the aquifer properties is rough and therefore, inhibits the spreading the plume. But due to the chaotic nature that is associated with the large fractal dimension, the behavior of the plume is not as predictable as anticipated in smaller fractal dimensions. Another significant finding relates to the scale dependence of the plume. The variance of $K$ over the plume thickness plays a major role in the spreading process. Larger the variance, larger is the asymptotic
It is stressed that the simulation attempts to model a simple scenario and further investigation needs to be done to encompass a more comprehensive, realistic flow systems. Several possibilities for additional work will involve 1) increasing the domain size, 2) inclusion of principal directions of hydraulic conductivity, 3) simulation of multispecies, and 4) inclusion of nonconservative solute.
Appendix A

Tables
<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t$</td>
<td>time</td>
<td>$[T]$</td>
</tr>
<tr>
<td>$x$</td>
<td>characteristic domain length</td>
<td>$[L]$</td>
</tr>
<tr>
<td>$C$</td>
<td>concentration of solute</td>
<td>$[ML^{-2}]$</td>
</tr>
<tr>
<td>$D_L$</td>
<td>longitudinal dispersion tensor</td>
<td>$[L^2T^{-1}]$</td>
</tr>
<tr>
<td>$D_T$</td>
<td>transversal dispersion tensor</td>
<td>$[L^2T^{-1}]$</td>
</tr>
<tr>
<td>$U$</td>
<td>Darcy flux</td>
<td>$[LT^{-1}]$</td>
</tr>
<tr>
<td>$K$</td>
<td>hydraulic conductivity</td>
<td>$[LT^{-1}]$</td>
</tr>
<tr>
<td>$n$</td>
<td>porosity</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$D$</td>
<td>fractal dimensions</td>
<td>dimensionless</td>
</tr>
<tr>
<td>$\alpha_T$</td>
<td>local transversal dispersivity</td>
<td>$[L]$</td>
</tr>
<tr>
<td>$\alpha_L$</td>
<td>local longitudinal dispersivity</td>
<td>$[L]$</td>
</tr>
</tbody>
</table>

Table A.1: Units for Main Variables

<table>
<thead>
<tr>
<th>D</th>
<th>Var(K) over $L_0$</th>
</tr>
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<tbody>
<tr>
<td>Run #1</td>
<td>1.1</td>
</tr>
<tr>
<td>Run #2</td>
<td>1.5</td>
</tr>
<tr>
<td>Run #3</td>
<td>1.9</td>
</tr>
<tr>
<td>Run #4</td>
<td>1.1</td>
</tr>
<tr>
<td>Run #5</td>
<td>1.5</td>
</tr>
<tr>
<td>Run #6</td>
<td>1.9</td>
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<tr>
<td>Run #7</td>
<td>1.1</td>
</tr>
<tr>
<td>Run #8</td>
<td>1.5</td>
</tr>
<tr>
<td>Run #9</td>
<td>1.9</td>
</tr>
</tbody>
</table>

Table A.2: List of Runs
Table A.3: Computed Values of $\text{Var}(K)$ over the Domain

<table>
<thead>
<tr>
<th>$D$</th>
<th>$\text{Var}(K)$ over $L_0$</th>
<th>$\text{Var}(K)$ over the Domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>100.0</td>
<td>6309.573</td>
</tr>
<tr>
<td>1.5</td>
<td>100.0</td>
<td>1000.000</td>
</tr>
<tr>
<td>1.9</td>
<td>100.0</td>
<td>158.489</td>
</tr>
<tr>
<td>1.1</td>
<td>625.0</td>
<td>39434.834</td>
</tr>
<tr>
<td>1.5</td>
<td>625.0</td>
<td>6250.0</td>
</tr>
<tr>
<td>1.9</td>
<td>625.0</td>
<td>990.558</td>
</tr>
<tr>
<td>1.1</td>
<td>900.0</td>
<td>56786.161</td>
</tr>
<tr>
<td>1.5</td>
<td>900.0</td>
<td>9000.000</td>
</tr>
<tr>
<td>1.9</td>
<td>900.0</td>
<td>1426.404</td>
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Table A.4: Comparison of $A_{\infty}$ and $A_N$

<table>
<thead>
<tr>
<th>$D$</th>
<th>$\text{Var}(K)$ over $L_0$</th>
<th>$K$</th>
<th>$\alpha_T$</th>
<th>$A_{\infty}$</th>
<th>$A_N$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>541.0378</td>
<td>0.00317950</td>
<td>0.0010179</td>
<td>0.0055771</td>
</tr>
<tr>
<td>1.5</td>
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<td>517.6200</td>
<td>0.00317950</td>
<td>0.0007826</td>
<td>0.0035080</td>
</tr>
<tr>
<td>1.9</td>
<td>100.0</td>
<td>507.4322</td>
<td>0.00317950</td>
<td>0.0002221</td>
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<tr>
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<td>0.0204173</td>
</tr>
<tr>
<td>1.5</td>
<td>625.0</td>
<td>544.0498</td>
<td>0.00317950</td>
<td>0.0044274</td>
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<tr>
<td>1.9</td>
<td>625.0</td>
<td>518.5836</td>
<td>0.00317950</td>
<td>0.0013290</td>
<td>0.0033355</td>
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<tr>
<td>1.1</td>
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<td>0.00317950</td>
<td>0.0069067</td>
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</tr>
<tr>
<td>1.5</td>
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<tr>
<td>1.9</td>
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<td>522.3000</td>
<td>0.00317950</td>
<td>0.0018866</td>
<td>0.0034272</td>
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</table>

Table A.3: Computed Values of $\text{Var}(K)$ over the Domain

Table A.4: Comparison of $A_{\infty}$ and $A_N$
<table>
<thead>
<tr>
<th>D</th>
<th>Var(K)</th>
<th>Slope</th>
<th>$D_L$</th>
<th>$V$</th>
<th>$A_N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
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<td>0.0069900</td>
<td>0.00349500</td>
<td>99.0228</td>
<td>0.005577086</td>
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<tr>
<td>1.5</td>
<td>100.0</td>
<td>0.0043961</td>
<td>0.002198036</td>
<td>99.0084</td>
<td>0.003507988</td>
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<tr>
<td>1.9</td>
<td>100.0</td>
<td>0.0040352</td>
<td>0.002017607</td>
<td>99.0064</td>
<td>0.003220095</td>
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<tr>
<td>1.1</td>
<td>625.0</td>
<td>0.0256120</td>
<td>0.012806002</td>
<td>99.1083</td>
<td>0.020417328</td>
</tr>
<tr>
<td>1.5</td>
<td>625.0</td>
<td>0.0064534</td>
<td>0.003226703</td>
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<td>1.9</td>
<td>625.0</td>
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<tr>
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<td>99.0114</td>
<td>0.003427222</td>
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</table>

Table A.5: Computation of $A_N$
Appendix B

Figures
Figure B.1: Perfectly Stratified Aquifer
Figure B.2: Concentration Contour of A Plume at a Later Stage of Transport
Second Moment Plot (D=1.5)

Figure B.3: Longitudinal Second Moment Plot for D=1.5
Numerical Macrodispersivity vs. Var(K)

Figure B.4: $A_N$ vs. Var(K)
Numerical Macrodispersivity vs. Fractal Dimension

Figure B.5: $A_N$ vs. Fractal Dimension, D
Bibliography


