GIS BASED STOCHASTIC MODELING OF GROUNDWATER SYSTEMS USING MONTE CARLO SIMULATION

By

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ABSTRACT

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Stochastic modeling of subsurface flow and transport has become a subject of wide interest and intensive research for last few decades and results evolution of many stochastic theories. These theories, however, have had relatively little impact on practical groundwater modeling. In a recent forum on stochastic subsurface hydrology: from theory to application, a number of leading experts in stochastic modeling stress that data limitation, the assumptions of linearization, stationarity, Gaussianity, and excessive computations required are the bottlenecks in practical stochastic modeling. These bottlenecks must be removed or substantially relaxed before stochastic modeling methods can be routinely applied in practice. Motivated by these critical assessments, this research addresses the issue of Gaussianity and issues of data limitations in stochastic modeling. The issue of Gaussianity is addressed by Monte Carlo Simulation (MCS). Data limitations issues are addressed using new source of Geographic Information Systems (GIS) database.

My first application considers a comprehensive study of synthetic scenarios to investigate the probabilistic structure of basic hydrogeological variables such as hydraulic head, groundwater velocity, concentration, seepage flux and solute flux. Results indicate that the statistical structure of groundwater systems in general non-Gaussian, nonstationary and anisotropic. Some critical state variables are extremely complex, with the probability distribution varying rapidly with locations and directions even for very weak heterogeneity. This study concludes that we can not always use variance as a good measure of uncertainty. Actual probability distribution from more

accurate and generalized method such as MCS is a better way to characterize the structure of hydrogeological variables. This research represents the first systematic analysis of the probabilistic structure of basic hydrogeological variables and findings from this work have significant implications on theoretical and practical stochastic subsurface hydrology.

My second application involves probabilistic delineation of well capture zones. In this paper, we explore the use of a recently-developed statewide GIS database in Michigan. We are particularly interested in exploring if the relatively crude, but detailed datasets can be used to characterize aquifer heterogeneity with sufficient details to enable practical stochastic modeling. We consider three approaches such as deterministic, stochastic macrodispersion, stochastic Monte Carlo, to delineate well capture zones, each representing a different way to conceptualize aquifer heterogeneity. Results show deterministic approach that accounts only for the effect of large-scale trend leads to capture zones that are significantly smaller than its stochastic counterpart. Stochastic Monte Carlo approach that models large-scale trends deterministically and small-scale heterogeneity as random field provides a probability map of well capture zone which is useful for risk-based decision making processes. Stochastic macrodispersion approach that models large-scale trends deterministically and small-scale heterogeneity as effective macrodispersion, provides a computationally efficient alternative to delineate well capture zones. A probability map of well capture zone has important implications for environmental policy on source water protection, risk management and sampling design.

DEDICATION

TO MY FAMILY

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PAPER 1

PROBABILISTIC STRUCTURE OF HYDROGEOLOGIC VARIABLES

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1.1 ABSTRACT

Most stochastic groundwater analyses rely on the critical assumption of Gaussianity for hydrogeological variables involved, although little is known systematically on their probabilistic structure. The conventional wisdom is – as long as the input source variability is not too strong and Gaussian, most dependent hydrogeological variables will be approximately normally distributed and a first-order method can be used to compute the first two statistical moments which can then be used to characterize the probabilistic distributions. This assumption is essentially the foundation of stochastic perturbation theory and the recent stochastic revolution that produced a huge body of literature on perturbation methods in the past three decades. Many researchers, however, question the validity of this assumption, stressing that the reliance on Gaussianity is one of the reasons stochastic methods are so difficult to apply in practice.

In this study, we investigate systematically the probabilistic structure of basic hydrogeological variables by performing an integrated analysis of groundwater flow and solute transport in heterogeneous media. In particular, we investigate the probabilistic distribution of hydraulic head, velocity, solute concentration, seepage flux, and solute flux, assuming hydraulic conductivity to be the source of uncertainty. We also investigate the effect of spatial integration on the probabilistic structure of seepage and solute fluxes. We consider both statistically uniform

and nonuniform flows for a range of situations, including weakly and strongly heterogeneous media, stationary and nonstationary media, and with and without aquifer stresses. We use the Monte Carlo approach to solve the stochastic groundwater flow and transport equations and make use of a recently-developed stochastic modeling software system. This software system is based on a new computing paradigm that enables real-time, parallel visual analysis and modeling of large numbers of realizations without storing them in memory or on disk, eliminating an implementation bottleneck in stochastic modeling. We observe and analyze the simulated probability distributions of interested variables throughout the computational domain at representative locations and of spatially integrated fluxes across transects of different lengths. We assess the Gaussianity of these probability distributions both visually and using the Q-Q plot technique. We also assess the feasibility to fit the simulated probabilities with empirical distribution under general conditions.

The following key findings emerge from this research:

- The statistical structure of a groundwater system under general, nonstationary condition is complex and cannot be characterized by a few simple statistical moments. Even when lnK is assumed to be Gaussian, the dependent hydrogeological variables can be strongly non-Gaussian, nonstationary, and for those that are directional, anisotropic.
- The closest to Gaussian, among all variables simulated, is the probability distribution of hydraulic head, when the scale of heterogeneity is much smaller than the domain size (e.g., 1/33 of the problem scale).
- The probability distribution of hydraulic head in response to larger scale heterogeneity (e.g., greater 1/10 of the problem scale) is often non-Gaussian and nonstationary and cannot be accurately fitted with a single functional distribution.

- The probability distribution of groundwater velocity is direction-dependent. The probabilistic structure of longitudinal velocity is strongly skewed.
- The probability distribution of transverse velocity is approximately Gaussian or symmetrically distributed, even in the presence of strong heterogeneity.
- Seepage flux across a transect representing integration of strongly skewed velocity, is approximately Gaussian, even in the presence of strong heterogeneity.
- Probability distribution of solute concentration is far from Gaussian and strongly nonstationary when the source size is relatively small (e.g., less than 10 lnK correlation scales), even for aquifers with very weak heterogeneity. The complex concentration probability distribution cannot be fitted with a single functional distribution.
- Solute flux across a transect, unlike its seepage flux counterpart, is strongly non-Gaussian and location-dependent.

This research represents the first comprehensive analysis of the probabilistic structure of basic hydrogeological variables and findings from this work have significant implications on theoretical and practical stochastic subsurface hydrology.

1.2 INTRODUCTION

Most stochastic groundwater analyses rely on the critical assumption of Gaussianity. The conventional wisdom is – as long as the source variability is not too strong and is Gaussian, most dependent hydrogeological variables would be approximately normally distributed. This is essentially the foundation of stochastic perturbation theory and the huge body of literature on

stochastic perturbation methods for flow and transport developed in the past three decades [Dagan, 1989; Gelhar, 1993; Cushman, 1997; Neuman, 1997; Zhang, 2001; Rubin, 2003]. Many researchers, however, question the validity of this assumption, stressing that the reliance on Gaussianity is one of the major reasons why stochastic methods are so difficult to apply in practice [Bellin et al., 1992a; Zhang and Neuman, 1995a-d; Hamed et al., 1996; Saladin and Fiorotto, 1998; Guadagnini and Neuman, 1999a,b; Zhang, 2001; Lu et al., 2002; Dagan, 2002; Li et al., 2003; Winter et al., 2003; Zhang and Zhang, 2004; Ginn, 2004; Neuman, 2004].

In a recent forum on stochastic subsurface hydrology: from theory to application, a number of leading experts in stochastic modeling stress that data limitation, the assumptions of linearization, stationarity, Gaussianity, and excessive computations required are the bottlenecks in practical stochastic modeling [Zhang and Zhang, 2004; Molz, 2004; Molz et al., 2004; Ginn, 2004; Winter, 2004; Neuman, 2004; Rubin, 2004; Dagan, 2004]

Experience from our own applications also shows that the observed variances of hydraulic head from linearized stochastic theories often cannot explain much of the observed variability in practical modeling. In fact, the observed variance in response to random, small-scale heterogeneity is almost negligible as compared to the uncertainty caused by errors in the representation of large scale variability, model conceptualization, and boundary conditions.

Gelhar [1993] stressed that the most significant effect of small-scale heterogeneity is on groundwater velocity and solute transport [Gelhar et al., 1979; Kapoor and Kitanidis, 1997; Salandin and Fiorotto, 2000; Darvini and Salandin, 2006; Morales-Casique et al., 2006a, 2006b].

In particular, Gelhar stressed that the observed variances from stochastic theories in groundwater velocity and solute concentration are much larger than that in hydraulic head. This strong sensitivity of solute transport to very small scale heterogeneity is in fact what attracted the recent explosion of research in stochastic subsurface hydrology. The significantly increased variance, however, is also what makes the application of stochastic perturbation theories problematic

Nowak et al. [2008] shows hydraulic heads in the presence of large scale heterogeneity can be non-Gaussian and approximated as beta distribution for statistically uniform flow between two constant head boundaries. Engler et al. [2006] shows that velocity in randomly heterogeneous media is approximately lognormal, with the skewness increasing with the variance of log hydraulic conductivity. Fiorotto and Caroni [2002], Caroni and Fiorotto [2005], Bellin and Tonina [2007] and Schwede et al. [2008] have studied the statistical distribution of concentration in a random heterogeneous medium and concluded that the probability density function of concentration follows approximately a beta distribution.

1.3 OBJECTIVE

In this study, we systematically investigate the probabilistic structure of basic hydrogeological variables. In particular, we investigate the probabilistic distributions of a complete set of basic dependent state variables - hydraulic head, velocity, solute concentration, and seepage flux and solute flux at a point and across a polyline. We assume log hydraulic conductivity is the only source of uncertainty and is normally distributed. The paper focuses on understanding how the nonlinear flow and transport equations transform the probability distributions of hydrogeological variables. This paper builds on several recent research that highlights the need to systematically

understand the probabilistic structure of hydrological variables [Engler et al., 2006; Fiorotto and Caroni, 2002; Caroni and Fiorotto, 2005; Bellin and Tonina, 2007; Nowak et al., 2008; Schwede et al., 2008].

Engler et al. [2006] stressed that with increasing variance of log hydraulic conductivity, the skewness and kurtosis of velocity components increases. This implies ignoring the actual shapes of the distributions may have severe consequences on the stochastic flow and transport theory.

The paper investigates the following important questions:

- 1. What is the probabilistic structure of commonly encountered hydrogeological variables in realistically complex groundwater systems?
- 2. Can the predicted variances of hydrogeological variables be used as an effective measure of uncertainty in groundwater modeling?
- 3. How does the scale of heterogeneity impact the probability distribution? How do the scale of variability and complex sources and sinks interact to control the probability distribution?
- 4. Is the head probability distribution approximately Gaussian? Under what conditions it can be assumed to be Gaussian?
- 5. What is the probability distribution of groundwater velocity and solute concentration? How do their probability distributions vary in space in a nonstationary flow system?
- 6. Does the probability distribution of groundwater velocity vary with direction?

- 7. Is aggregated probability distribution of seepage flux across a polyline more Gaussian? How does the scale of integration affect the probability distributions of seepage flux?
- 8. What is the probability distribution of solute fluxes?

1.4 APPROACH

To address these questions systematically, we perform a comprehensive Monte Carlo simulation exercise involving integrated flow and transport modeling. This simulation exercise is conceptually straightforward, but the results, as we will show further on, have significant implications and provide very useful insights for practical stochastic groundwater modeling. We consider a range of modeling scenarios in this exercise, including

- weakly and strongly heterogeneous media;
- stationary and nonstationary media;
- with and without external stresses.

We make use of a recently-developed modeling software system, Interactive Groundwater (IGW) [Li and Liu, 2003, 2006; Li et al., 2006] to solve the stochastic groundwater flow and transport equations. This software system differs from a traditional one in that it allows real-time, parallel analysis and visualization of model statistics and probabilities, enabling simulating large numbers of realizations for a range of modeling scenarios. The software also allows stochastic simulations without simultaneously storing them in memory or on disk, eliminating an implementation bottleneck in stochastic modeling.

We monitor, analyze, and compare the probability distributions of interested key state variables at representative locations throughout the simulation domain. We assess the Gaussianity of these probability distributions both visually and using the Q-Q plot technique [Chambers et al., 1983] We also assess the feasibility to fit the simulated probabilities with a general empirical distribution.

In a Q-Q (Quantile-Quantile) plot, the quantiles of dependent variable from the Monte Carlo simulation are plotted against the quantiles of a standard normal distribution. A straight line implies that the distribution is a normal distribution. Any deviation from the straight line is the indication of deviation from the normality.

1.5 PROBLEM DESIGN

We consider two dimensional steady state flows in confined aquifer. Figure 1.1 shows the model domain, boundary conditions, aquifer stresses, and monitoring network. We develop numerical models with no flow boundary conditions along north and south boundaries and constant heads along east and west boundaries.

A constant head of 2 m is assigned to west boundary and 0 (zero) m to east boundary. The domain size is 1000 m x 750 m. A source of constant recharge of 0.001 m/day, two pumping wells, and statistically nonstationary conductivity zones are also introduced in some modeling scenarios. A contaminant plume is injected from the west side of the model. The plume source is continuous with concentration of 100 ppm (mg/L) spanning across twice the length of correlation scale of log hydraulic conductivity.



Figure 1.1: Model domain showing locations of monitoring wells, polylines (each polyline is a set of two polylines as shown in extreme right of the figure), pumping wells, plume source and different conductivity zones, Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day). Zone 1 and Zone 2 are shown in shaded areas. For interpretation of the references to color in this and all other figures, the reader is referred to the electronic version of this thesis (or dissertation).

To investigate the probabilistic structure of hydrogeological variables, we consider four different simulation scenarios, as shown in Table 1.1.

	Case 1, Stationary flow, low lnK variance	Case 2, Stationary flow, high lnK variance	Case 3, nonstationary flow, nonstationary lnK variances	Case 4, nonstationary flow, with pumping
Domain length (m)	1000 x 750	1000 x 750	1000 x 750	1000 x 750
West boundary condition	Constant Head	Constant Head	Constant Head	Constant Head
East boundary condition	Constant Head	Constant Head	Constant Head	Constant Head
North boundary condition	No Flow	No Flow	No Flow	No Flow
South boundary condition	No Flow	No Flow	No Flow	No Flow
Global Recharge(m/day)	0.001	0.001	0.001	0.001
Number of wells	0	0	0	2
Geometric mean conductivity (K _G) (m/day)	100	100	2,20,200	2,20,200
LnK correlation scales $(\lambda)(m)$	30	30	2, 10, 20	2, 10, 20
Ln K Variance (σ_{Y}^2)	0.1	2	0.5, 1.5, 3	0.5, 1.5, 3

Table 1.1: Parameter Definitions for four cases

The first two cases consider a stationary system with a variance of 0.1 (weakly heterogeneous) and 2.0 (strongly heterogeneous) for log hydraulic conductivity, respectively. The third and fourth cases involve nonstationary systems with three different hydraulic conductivity zones and pumping wells, respectively.

The lnK variances used reflect the range of variability observed in real-world sites. The well known Cape Cod site in Massachusetts is relatively homogeneous and has lnK variance of 0.24. The popular Columbus research site in Mississippi is strongly heterogeneous and has lnK variance of 4.5 [Gelhar, 1993]

Monitoring wells are distributed in a grid format of 5 rows and 6 columns (total of 30) to observe the probability distributions of hydraulic head, longitudinal velocity, transverse velocity and concentration (Figure 1.1). Groups of polylines at seven different locations perpendicular to the flow direction are used to observe the probability distributions of integrated seepage and solute fluxes. Within each group, polylines of two different lengths [see Figure 1.1, extreme right numbered as 1 and 2] are used to investigate the effect of scale of integration on the shape of probability distributions of seepage and solute fluxes.

Monte Carlo Simulation: The MC simulation is carried out in three steps:

Random Field Generation: This step creates realizations of random hydraulic conductivity. The random field of hydraulic conductivity is generated using a Fast Fourier Transform-based spectral algorithm. The exponential covariance model [Gelhar and Axness, 1983; Gelhar, 1986;

Dagan, 1994; Ni and Li, 2005, 2006] is used to describe the spatial structure of hydraulic conductivity.

Numerical Solution: For a given realization, the governing equations become deterministic and are solved by central finite difference methods for groundwater flow and the modified methods of characteristics for solute transport. Discretization cell sizes are designed such that the scale of heterogeneity can be resolved [Li et al. 2003, 2004].

Statistical Postprocessing: Once the realizations are solved, the solution of flow and transport quantities such as hydraulic head, velocity, concentration and fluxes are processed to compute statistical moments and probability distributions. The statistical moments and probability distribution of hydraulic head at points of interest are computed by

$$\langle h(x) \rangle_{s} = \frac{1}{N} \sum_{n=1}^{N} h_{n}(x)$$
 (1.1)

$$Var[h(x)]_{s} = \frac{1}{N} \sum_{n=1}^{N} [h_{n}(x) - \langle h(x) \rangle_{s}]^{2}$$
(1.2)

Here N is the total number of realizations and $h_n(x)$ is the head at x from nth realization. The

covariance of head at the points x and x_1 is computed by

$$Cov[h(x),h(x_1)]_{S} = \frac{1}{N} \sum_{n=1}^{N} h_n(x)h_n(x_1) - \langle h(x) \rangle_{S} \langle h(x_1) \rangle_{S} \quad (1.3)$$

The probability distribution is computed by:

$$p(h_j) = n_j/N, \quad j = 1, 2, ..., M$$
 (1.4)

where n_j is the total number times the simulated head values fall into the interval $[h_j, h_j+1]$, *M* is the number of interval the entire range of simulated heads are divided into, and

$$M$$

$$\sum_{j=1}^{N} n_j = N$$

$$j=1$$

$$h_j = h_{min} + j (h_{max} - h_{min}) / M,$$

The symbols h_{min} and h_{max} are respectively the minimum and maximum head values at the monitoring point.

The accuracy of Monte Carlo simulation depends on the number of realizations. The number of realizations is selected to ensure that the observed probability distributions stabilize. The number of realizations used in this simulation exercise is generally in the range of 5000- 6000.

1.6 RESULTS AND DISCUSSION

Modeling results are summarized in Figures 1.2 through 1.13. Selected Q-Q plots are shown in Figures 1.14 through 1.19. Additional information on the distribution statistics (skewness and kurtosis) are presented in Table 1.2 -1.7 in the Appendix.

The results from Monte Carlo simulation clearly show that probability distribution of hydrogeological variables is, in general, non-Gaussian, nonstationary, and cannot be described by the first two statistical moments or a predefined distribution function based on these statistical moments. The probability distribution can vary structurally from variable to variable and location to location. The probability distributions of solute concentration and concentration fluxes are particularly complex, departing sharply from Gaussian distribution and varying strongly and rapidly with locations even for weakly heterogeneous conductivity fields.

The following is a variable by variable discussion of the probability structure for all scenarios considered.

Hydraulic Head

Figures 1.2-1.4 show the observed probability distribution of hydraulic head for different cases. The results show that the probability distribution of hydraulic head, among all dependent variables, is the closest to Gaussian. The exceptions are in areas close to pumping well and boundary conditions.

Figures 1.2 to Figure 1.4a show that probability distributions of hydraulic head when the scale of lnK heterogeneity is 1/33 of the simulation domain. The simulated probability distributions at

most locations are approximately Gaussian. The Q-Q plot in Figure 1.14 shows a straight line, indicating normality.

The gaussianity of the head can be attributed to the fact that head at steady state depends on log conductivity, not conductivity itself, and the transformation between lnK fluctuation and head fluctuation is almost linear in areas where mean hydraulic gradient is small, especially when the scale of heterogeneity is also relatively small.

For the high variance case, the probability distributions of hydraulic head at locations near the constant head boundaries (e.g., MW3, MW28) are slightly skewed towards the constant head values specified on the boundaries. The Q-Q plot of hydraulic head (see Appendix, Figure 1.14) at these locations shows a departure from the straight line, indicating local non-Gaussianity.

Figure 1.3 shows the presence of the three conductivity zones alters the hydraulic gradient, head variance, and probability distribution, but not much in the shape of the probability distributions. The Q-Q plots for these probability distributions still show a straight line, indicating normality.

Figures 1.4ab shows pumping can impact significantly the shape of the probability distribution of hydraulic head, especially in the proximity of the pumping well. The probability distributions of head become skewed in the area where there is significant drawdown.

Figure 1.4b shows that the probability distributions for hydraulic head close to the pumping well are also strongly nonstationary in space.

Figure 1.4c shows the probability distribution of hydraulic head when the scale of heterogeneity is increased to 1/10 of the simulation domain. Large-scale heterogeneity results clearly more

non-Gaussian behavior, which in turn may result a non-Gaussian distribution on other dependent variables. The shape of probability distributions becomes more complex and is influenced more by boundary conditions, nonstationary conductivity distribution, and the presence of sources and sinks.



Figure 1.2: Probability distributions of hydraulic head for stationary cases (Top: lnK variance =0.1, Bottom: lnK variance =2.0). Black circles are monitoring wells and thin solid lines are head contours in the model domain.



Figure 1.3: Probability distributions of hydraulic head for Nonstationary case without pumping wells (Zone 1(lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and thin solid lines are head contours in the model domain.



Figure 1.4a: Probability distributions of hydraulic head for Nonstationary case with pumping wells (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and thin solid lines are head contours in the model domain.



Figure 1.4b: Probability distributions of hydraulic head observed close to the pumping well. Black circles are monitoring wells and thin solid lines are the head contours in the model domain.



Figure 1.4c: Probability distributions of hydraulic head for Nonstationary case with pumping wells having large correlation scale (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and thin solid lines are head contours in the model domain.

Velocity

Figures 1.5-1.7 show the observed probability distribution of groundwater velocity for different cases. It is interesting to note that probability distributions of longitudinal velocity and transverse velocity are structurally different.

Figure 1.5a shows that the probability distribution of longitudinal velocity at low lnK variance is slightly asymmetric, but becomes strongly skewed at the higher lnK variance of 2.0. The Q-Q plot of longitudinal velocity (see Appendix, Figure 1.15) indicates that even at low variance the quantiles of longitudinal velocity deviates from the straight line and, as the lnK variance increases, the deviation becomes more prominent.

The skewness in the velocity probability distribution can be directly attributed to the fact that velocity is proportional to hydraulic conductivity and its variability is dominated by the variability in hydraulic conductivity. Since hydraulic conductivity is assumed to be lognormal, the longitudinal velocity is expected to be strongly skewed.

Figure 1.5b shows that the probability distribution of transverse velocity is interestingly always symmetrically distributed, even in the presence of strong heterogeneity. At a low lnK variance, the corresponding Q-Q plot (see Appendix, Figure 1.16) closely matches with the theoretical straight line, indicating normality.

For strongly heterogeneous media at high lnK variance of 2.0, the Q-Q plot shows deviation from the theoretical straight line, implying that the distribution, though symmetrical, is non-Gaussian (see Appendix, Figure 1.16).

Figures 1.6ab and 1.7ab show that the probability distributions of velocity in a particular direction in a nonstationary flow system are strongly nonstationary. As the direction of flow changes the shapes of the probability distributions in X-velocity and Y-velocity change significantly.

However, if we focus our attention on the longitudinal and transverse velocities, their probability distributions change little with location and are not particularly sensitive to boundary conditions, aquifer stresses and other sources and sinks.



Figure 1.5a: Probability distributions of X-velocity for stationary cases (Top: lnK variance =0.1, Bottom: lnK variance =2.0). Black circles are monitoring wells and thin solid lines are head contours in the model domain.



Figure 1.5b: Probability distributions of Y-velocity for stationary cases (Top: lnK variance =0.1. Bottom: lnK variance =2.0). Black circles are monitoring wells and thin solid lines are head contours in the model domain.



Figure 1.6a: Probability distributions of X-Velocity for Nonstationary case without pumping wells (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and thin solid lines are head contours in the model domain.


Figure 1.6b: Probability distributions of Y-Velocity for Nonstationary case without pumping wells (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and thin solid lines are head contours in the model domain.



Figure 1.7a: Probability distributions of X-Velocity for Nonstationary case with pumping wells (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and thin solid lines are head contours in the model domain.



Figure 1.7b: Probability distributions of Y-Velocity for Nonstationary case with pumping wells (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and thin solid lines are head contours in the model domain.

Concentration

Figures 1.8-1.9 show the observed probability distribution of solute concentration for both stationary and nonstationary flow cases. The results show that concentration probability distributions are the most complex, strongly non-Gaussian and nonstationary in both space and time even for lnK variance of 0.1. The Q-Q plot of concentration (see Appendix, Figure 1.17) show that simulated concentration probability distribution deviates substantially from the theoretical normal distribution.

The results also show that the complex concentration probability structure can be best characterized based on its relative location to the mean plume. In particular, both for uniform and non-uniform flow situations, the results show that the concentration probability distributions at locations close to the source concentration (the specified source concentration is 100 ppm) are strongly skewed right. The probability distributions at locations within the mean plume is strongly skewed toward the left or zero. The distributions at locations within the mean plume represent a transition between the two extreme distributions.

Because of the extremely skewed nature in concentration probability, variance provides little information on concentration uncertainty and it is impractical fit accurately the highly nonstationary probability distribution using a predefined function.



Figure 1.8: Probability distributions of concentration for Stationary case. Black circles are monitoring wells and the color contours are the concentration.



Figure 1.9: Probability distributions of concentration for Nonstationary case (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Black circles are monitoring wells and the color contours are the concentration.

Seepage flux across a polyline

Figures 1.10-1.11 present the observed probability distribution of seepage flux for different cases. The results show that the probability distributions of seepage flux is approximately Gaussian at low variance when it is integrated along a polyline. As the variance of lnK increases, the probability distributions of seepage flux become more non-Gaussian, but its skewness is less extreme than that in the original velocity.

Spatial integration has the effect of reducing variability, rendering the transformation from lnK fluctuation to flux fluctuation more linear.

Figure 1.18 shows that the seepage flux quantiles deviate from the theoretical straight line at high variance, indicating non-Gaussianity.

Overall, the shapes of the seepage flux distributions depend on the scale of integration along the polyline and on degree of heterogeneity. The probability distribution of the seepage flux becomes more Gaussian as the scale of integration increases or as lnK variance decreases.



Figure 1.10: Probability distributions of seepage flux for stationary cases at each polylines. Thick solid lines represent the length of the polylines and thin solid lines are the head contours in the model domain. Top: lnK variance =0.1, Bottom: lnK variance =2.0.



Figure 1.11: Probability distributions of seepage flux at each polylines for nonstationary case with pumping wells (Zone 1 (lnK variance =0.5, λ = 2m, K= 2m/day), Zone 2 (lnK variance =3.0, λ = 20m, K= 200m/day) and Zone3 (lnK variance =1.5, λ = 10m, K= 20m/day)). Thick solid lines represent the length of the polylines and thin solid lines are the head contours in the model domain.

Solute Flux across a Polyline

Figures 1.12-1.13 present the observed probability distribution of solute flux for different cases. The results show that the probability distribution of integrated solute flux is non-Gaussian except when lnK variance is very small.

At a low lnK variance of 0.1, solute flux is slightly skewed, and the Q-Q plot in Figure 1.19 shows a slight departure from the theoretical straight line of normality.

However, as lnK variance increases, the probability distributions in solute flux become strongly skewed, though less extreme than the original concentration probability distribution because of spatial integration.

In general, the skewness of the distribution for solute flux across a polyline increases as the length of the polyline decreases and the degree of heterogeneity increases (see Appendix, Figure 1.19).

Because of the strongly skewed nature of solute flux, variance in its distribution provides little information on uncertainty and it is impractical fit accurately the highly nonstationary probability distribution using a predefined function.



Figure 1.12: Probability distributions of solute flux at each polylines for Stationary case. Thick solid lines represent the length of the polylines and the color contours are the concentration.



Figure 1.13: Probability distributions of solute flux at each polylines for Stationary case. Thick solid lines represent the length of the polylines and the color contours are the concentration.

1.7 CONCLUSIONS

The following key findings emerge from this research:

- The statistical structure of a groundwater system under general, nonstationary condition is complex and cannot be characterized by a few simple statistical moments. Even when lnK is assumed to be Gaussian, the dependent hydrogeological variables can be strongly nongaussian, nonstationary, and for those that are directional, anisotropic.
- The closest to Gaussian, among all variables simulated, is the probability distribution of hydraulic head, when the scale of heterogeneity is much smaller than the domain size (e.g., 1/33of the problem scale).
- The probability distribution of hydraulic head in response to larger scale heterogeneity (e.g., greater 1/10 of the problem scale) is often non-Gaussian and nonstationary and cannot be accurately fitted with a single functional distribution.
- The probability distribution of groundwater velocity is direction-dependent. The probabilistic structure of longitudinal velocity is strongly skewed.
- The probability distribution of transverse velocity is approximately Gaussian or symmetrically distributed, even in the presence of strong heterogeneity.
- Seepage flux across a transect representing integration of strongly skewed velocity, is approximately Gaussian, even in the presence of strong heterogeneity.
- Probability distribution of solute concentration is far from Gaussian and strongly nonstationary when the source size is relatively small (e.g., less than 10 lnK correlation

scales), even for aquifers with very weak heterogeneity. The complex concentration probability distribution cannot be fitted with a single functional distribution.

• Solute flux across a transect, unlike its seepage flux counterpart, is strongly non-Gaussian and location-dependent.

This research represents the first comprehensive analysis of the probabilistic structure of basic hydrogeological variables and findings from this work have significant implications on theoretical and practical stochastic subsurface hydrology.

APPENDIX

APPENDIX

STATISTICAL PARAMETERS OF GROUNDWATER VARIABLES

Table 1.2:	Statistical parameters (Skewness and Kurtosis)of Head, X-Velocity and Y-
	velocity for low and high lnK Variances

TTJ								
Head								
	MW3		MW13		MW28			
-	Skewness	Kurtosis	Skewness Kurtosis		Skewness	Kurtosis		
lnK variance=0.1	-0.04	-0.05	-0.04	-0.01	0.04	0.05		
lnK variance=2.0	-0.54	0.45	-0.06	-0.17	0.54	0.45		
Nonstationary without pumping	-0.16	-0.09	0.11	0.11	0.12	0.02		
well								
X-Velocity								
			-					
lnK variance=0.1	0.51	0.49	0.46	0.29	0.51	0.49		
lnK variance=2.0	2.32	9.76	2.38	10.10	2.32	9.76		
Nonstationary	0.64	0.67	1.78	5.08	2.09	6.31		
without pumping								
well								
Y-Velocity								
lnK variance=0.1	0.04	0.29	-0.00	0.42	-0.04	0.29		
lnK variance=2.0	-0.25	10.77	0.17	6.66	0.25	10.77		
Nonstationary	-0.50	0.60	1.25	4.23	0.07	9.59		
without pumping								
well								

	Head		X-Velocity		Y-Velocity	
	Skewness	Kurtosis	Skewness	Kurtosis	Skewness	Kurtos is
MW3	-0.18	-0.07	0.70	0.95	-0.51	0.64
MW13	0.19	0.13	1.65	4.34	1.60	6.26
MW18	-0.01	0.22	2.09	6.50	1.86	10.48
MW23	-0.67	1.59	-1.96	5.47	1.78	7.74
MW28	-0.23	0.07	-2.31	8.10	1.23	10.17

Table 1.3 : Statistical parameters (Skewness and Kurtosis)of Head, X-Velocity and Y-Velocity for Nonstationary with pumping wells

Table 1.4: Statistical parameters (Skewness and Kurtosis)of Head, for Nonstationary with pumping wells having large scale heterogeneity

Head						
	Skewness	Kurtosis				
MW3	-0.67	0.40				
MW13	-0.12	0.88				
MW18	-0.50	2.59				
MW23	-0.77	3.37				
MW28	-1.11	4.73				

Table 1.5: Statistical parameters of Head in the sub model domain for nonstationary case with pumping well

	MW2	MW7	MW9	MW20	MW23
Skewness	-5.76	-1.45	-1.39	-0.64	-1.23
Kurtosis	49.12	4.45	5.40	0.39	4.09

lnK variance=0.1			Non stationary with pumping well			
	Skewness	Kurtosis		Skewness	Kurtosis	
MW5	-6.20	57.17	MW3	2.02	6.03	
MW12	1.57	2.28	MW4	-0.07	-1.04	
MW14	3.63	19.27	MW5	9.92	147.59	
MW18	-0.84	-0.04	MW8	13.32	276.68	
MW19	2.18	5.95	MW9	1.11	0.69	
MW23	2.18	4.95	MW13	5.08	33.63	

Table 1.6 : Statistical parameters (Skewness and Kurtosis) of ConcentrationFor low variance of lnK and for nonstationary case with pumping wells

Table 1.7: Statistical parameters (Skewness and Kurtosis)of seepage and solute fluxes For low and high lnK variances

	Seepage Flux		Solute Flux			
	PL1	PL2	PL1	PL2	PL5	PL6
Skewness (lnK variance=0.1)	0.06	0.40	0.26	0.40	0.23	0.04
Kurtosis (lnK variance=0.1)	-0.12	0.31	0.08	0.29	0.19	0.21
Skewness (lnK variance=2.0)	0.36	1.86	1.18	1.92	1.01	2.22
Kurtosis (lnK variance=2.0)	0.16	5.68	2.30	6.20	1.46	8.15

QUANTILES-QUANTILES PLOTS

Q-Q Plot of Hydraulic Head versus Standard Normal Distribution



Figure 1.14: Q-Q plot of Hydraulic head data versus normal distribution for low variance and high variance cases. MW3: located near the west boundary, MW28: Located near the east boundary, MW13: located approximately middle of the model domain.

Q-Q Plot of Hydraulic Head versus Standard Normal Distribution



Figure 1.14 (cont'd).

Q-Q Plot of Hydraulic Head versus Standard Normal Distribution



Figure 1.14 (cont'd).



Figure 1.14 (cont'd).





Figure 1.14 (cont'd).



Figure 1.14 (cont'd).



Figure 1.15: Q-Q plot of X-Velocity data versus normal distribution for low and high lnK variance





Figure 1.15 (cont'd).



Figure 1.16: Q-Q plot of Y-Velocity data versus normal distribution for low and high lnK variance





Figure 1.16 (cont'd).

Q-Q Plot of Concentration versus Standard Normal Distribution



Figure 1.17: Q-Q plot of concentration data versus normal distribution



Q-Q Plot of Concentration versus Standard Normal Distribution

Standard Normal Quantiles

Figure 1.17 (cont'd).





Figure 1.18: Q-Q plot of seepage flux data versus normal distribution for low and high lnK variance



Figure 1.18 (cont'd).





Figure 1.18 (cont'd)

Q-Q Plot of Seepage Flux versus Standard Normal Distribution



Figure 1.18 (cont'd).

Q-Q Plot of Solute Flux versus Standard Normal Distribution



Figure 1.19: Q-Q plot of solute flux data versus normal distribution for low and high lnK variance



Figure 1.19 (cont'd).


Figure 1.19 (cont'd).



Standard Normal Quantiles

Figure 1.19 (cont'd).

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PAPER 2

PROBABILISTIC WELL CAPTURE ZONE DELINEATION USING A STATEWIDE GROUNDWATER DATABASE SYSTEM

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2.1 ABSTRACT

It is widely known that data limitation is a major practical bottleneck in stochastic groundwater modeling. An expert panel at a recent forum on the state of practice in stochastic subsurface modeling and hydrology suggested that new measurement technologies or data sources of much better resolution are needed if we are to enable routine application of stochastic methods in real world investigations.

In this paper, we explore the use of a recently-developed statewide database in Michigan for stochastic groundwater modeling and apply it to probabilistic capture zone delineation. We are particularly interested in testing if the relatively crude, but detailed datasets can be used to characterize aquifer heterogeneity with sufficient details to enable practical stochastic modeling in the context of source water protection. This research represents an extension of our earlier work that uses this data source for basic deterministic modeling and cost effective source water management in Michigan. Our earlier research clearly shows that this new data source, despite its significant uncertainty, is effective in modeling regional mean flow patterns, directions and particularly source water protection areas. Our earlier research also shows that capture zone delineation based on regional patterns without taking into account smaller scale heterogeneity

can significantly underestimate the size of capture zone. As a pragmatic way to improve the delineation, managers and practitioners often manually draw a "grey area" around "skinny" capture zones to account for the effect of un-modeled heterogeneity.

We attempt in this research to quantify these grey areas probabilistically in a systematic manner. In particular, we consider the following four approaches to delineate well capture zones, each representing a different way to conceptualize aquifer heterogeneity.

- Deterministic approach: modeling large scale heterogeneity as a deterministic trend, ignoring the uncertainty in large-scale heterogeneity and the effect of small scale heterogeneity;
- Stochastic unconditional method: modeling heterogeneity as a random field using Monte Carlo simulation;
- Stochastic semiconditional method: modeling large scale heterogeneity as a deterministic trend and smaller scale heterogeneity as a random field using unconditional Monte Carlo simulation;
- Stochastic macrodispersion method: modeling large-scale heterogeneity as a deterministic trend and small scale heterogeneity deterministically using effective macrodispersion.

These approaches were applied to several selected sites with distinct characteristics to delineate well capture zones. The results are systematically analyzed and compared. The following findings emerge from this research:

- A significant portion of the variability in the statewide conductivity dataset is uncorrelated noise and this data noise can be quantified through variogram modeling.
- Despite the data noise, two scales of natural variability in conductivity can be identified;

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- Kriging based on the large-scale variograms, with small scale variability and data noises represented as nuggets, can be used to delineate large scale trends.
- Variogram modeling of detrended conductivity data can be used to identify smaller scale heterogeneity. The residual variograms are significantly noisier, but statistically meaningful structures can be detected;
- Deterministic delineation that accounts only for the effect of large scale trend leads to capture zones that are significantly smaller than its stochastic counterpart, especially in areas where regional gradient is relatively strong;
- Stochastic Monte Carlo simulation provides a map of well capture probability. Combined with the statewide database, MC provides a useful, systematic tool for risk-based decision making;
- Stochastic macrodispersion method provides a computationally efficient alternative to delineate wellhead protection area in a way that accounts for the effect of both small and large scale heterogeneity.

Future research should focus on 3D stochastic modeling using 3D lithology and calibrating the conductivity to statewide static water level dataset.

2.2 MOTIVATION AND OBJECTIVE

It is widely known that data limitation is a major practical bottleneck in stochastic groundwater modeling. An expert panel at a recent forum on the state of practice in stochastic subsurface modeling and hydrology suggested that new measurement technologies or data sources of much better resolution are needed if we are to enable routine application of stochastic methods in real world investigations [Dagan, 2002; Harrar et al., 2003; Zheng and Gorelick, 2003; Molz et al., 2003; Zhang and Zhang 2004; Winter, 2004; Dagan 2004; Neuman, 2004; Molz, 2004].

In this paper, we explore the use of a recently-developed statewide database system in Michigan [GWIM, 2006; Wellogic, 2006; Map Image viewer, RS&GIS-MSU] for stochastic groundwater modeling and apply it to probabilistic well capture zone delineation. We are particularly interested in exploring if the relatively crude, but detailed water well records can be used to characterize aquifer heterogeneity with sufficient details to enable practical stochastic modeling in the context of source water protection. This research represents an extension of earlier work that used this database for basic deterministic modeling and improved source water management [Simard, 2007; Li et al., 2009; Oztan, 2010]. This earlier research clearly showed that this new data source, despite its significant uncertainty, is effective in modeling regional mean flow patterns, flow directions and particularly source water protection areas. This earlier research also showed that capture zone delineation based on regional patterns without taking into account smaller scale heterogeneity can significantly underestimate the size of well capture zone.

The significant effect of heterogeneity on groundwater flow and transport has been widely recognized and an area of intense research in past decades [Dagan, 1989; Gelhar 1993; Rubin, 2003]. Variability in aquifer properties translates into uncertainty in groundwater seepage velocity, which in turn causes uncertainty in contaminant transport. A number of researchers recently stressed that spatial variability of aquifer properties (e.g., hydraulic conductivity) is one of the main sources of uncertainty in capture zone delineation [e.g., Varljen and Shafer, 1991; Wheater et al., 1998; van Leeuwen et al., 1998; Feyen et al., 2001; Stauffer et al., 2002; Feyen et al., 2003; Hendricks Franssen et al., 2004b; Stauffer et al., 2005] and have used stochastic

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approaches to model well capture zone areas [Varljen and Shafer, 1991; Bair et al., 1991; Vassolo et al., 1998; van Leeuwen et al., 2000; Feyen et al., 2001]. A stochastic approach simulates uncertain, heterogeneous input parameter fields as random fields and allows modeling not only the area of well capture but also the probability of capture, providing a systematic, risk-based framework for decision making [e.g., Franzetti and Guadagnini, 1996; Guadagnini and Franzetti, 1999; Riva et al., 1999; Delhomme, 1978, 1979; Varljen and Shafer, 1991; van Leeuwen et al., 1998, 1999; Starn et al., 2000; Van Leeuwen et al., 2000; Riva et al., 2006].

The Achilles' heel of stochastic approaches, however, is their intensive data requirements [Dagan, 2002; Harrar et al., 2003; Zhang and Zhang 2004, Winter, 2004; Dagan 2004; Neuman, 2004; Molz, 2004]. Unlike deterministic modeling, stochastic approaches require not only characterizing the means of input fields but also modeling their variogram structures to estimate the geostatistical parameters. Datasets allowing such estimation are often very difficult to obtain in practice.

A literature review on stochastic groundwater modeling over the years shows that stochastic approaches are rarely used outside of research applications [Harrar et al., 2003]. In particular, the review shows current efforts in stochastic capture zone modeling suffer from the following limitations:

 The vast majority of the stochastic modeling studies focus on hypothetical sites; assuming known statistical structure of small-scale heterogeneity [e.g., Varljen and Shafer 1991; Cole 1995; Franzetti and Guadagnini, 1996; Kinzelbach et al., 1996; Cole and Silliman, 1996; van Leeuwen et al., 1998; Hendricks Franssen et al., 2004b].

- Among the relatively few site-specific, real-world applications, the datasets used are often highly limited too sparse to reliably characterize real world heterogeneity [e.g., Johanson, 1992; Vassolo et al., 1998; Riva et al., 2006; Theodossiou et al., 2005]. Because of this, as Gelhar [1993], stressed there is often significant uncertainty about predicted uncertainty in stochastic modeling.
- 3. While the original motivation of stochastic modeling was to enable better coping with complex realities, most of the newly developed stochastic methods (e.g., perturbation methods) apply only for simple, statistically uniform processes, free of complex sources and sinks, boundary conditions, and nonstationarities [Li and McLaughlin, 1993, 1995; Li, Liao and Ni, 2004].
- Some of the stochastic methods developed only allow representing uncertain aquifer properties or stresses as random constants [e.g., Evers and Lerner, 1998, Kinzelbach et al., 1996].

Future direction of stochastic subsurface hydrology research should clearly focus on the development of approaches, data sources, or measurement technologies that allow modeling problems of realistic sizes and complexities [Zhang and Zhang, 2004; Ginn, 2004; Neuman, 2004]. Stochastic methods need data of good resolution and must allow modeling both large-scale (systematic) and small-scale (random) heterogeneity and stresses before they can become routine tools for practical applications.

2.3 DATA INTENSIVE STATEWIDE MODELING SYSTEM

Over the past decade, the Michigan Department of Natural Resources and Environment (DNRE) has in a major statewide data integration effort, capitalizing on the recent dramatic engaged developments in remote sensing, Global Position System (GPS), and Geographic Information System (GIS) technologies. In this process, the DNRE has created a statewide GIS-based groundwater database system [Wellogic, 2006; GWIM, 2006; Map Image viewer, RS&GIS-MSU] that can be used to model regional scale processes and potentially local flow systems. The network of databases contains virtually "all" data needed for typical groundwater flow simulations [Li et al., 2009]. In particular, the databases contain data for defining model areas (e.g., watershed delineations, the Great Lakes, streams, and inland lakes), aquifer elevations (e.g., digital elevation model - DEM, lithologies), aquifer properties (e.g., lithologies, specific capacities), aquifer heterogeneity (lithologies, glacial land systems), aquifer stresses (e.g., estimated recharge, streams, lakes, wetlands, drains, and wells), surface water levels (e.g., DEM), contamination sources (e.g., industrial sites, landfills, leaky underground storage tanks), as well as, data for model calibration (e.g., static water levels, estimated baseflows, aquifer test hydrographs, and hydrographs from long term USGS monitoring wells).

To enable systematic use of this vast "new" data source, Li et al. [2009] have recently developed an intelligent link between the databases and a real-time hierarchical groundwater modeling system [Li and Liu, 2006, 2008; Li et al., 2009]. The result is a data-intensive, statewide platform that can be used to model groundwater flow virtually anywhere (the areas covered by the database) in Michigan's aquifers. The modeling system is "live-linked" in a hierarchical fashion to Michigan's streams, lakes, geology, and water wells.

The hierarchical modeling system simulates state's two uppermost aquifer layers – the glacial drift aquifer and/or the bedrock aquifer. Aquifer elevations are defined based on approximately half a million of well logs, including logs from water wells, as well as, oil and gas wells. Hydraulic properties are estimated using more than 300,000 water well records, including test pumping information and lithologic descriptions. Natural recharge to the glacial aquifer is estimated using data on land use, soil conditions, watershed characteristics, and observed stream flow hydrographs at more than 400 gaging stations statewide [GWIM,2006]. The Great Lakes are represented in the glacial aquifer as prescribed heads equal to the long term average of observed lake levels. Large inland lakes and rivers are represented as head-dependent fluxes. Wetlands, ponds, small lakes, and small streams are treated by default as drains. A default leakance value is assigned to all lakes, wetlands, and stream arcs based on the 10 to 30 m statewide DEM. All default representations and parameter values in the modeling system can be interactively modified.

The estimation of hydraulic conductivity in the database is briefly presented below.

Hydraulic Conductivity:

The horizontal hydraulic conductivity in the database was calculated from water well records using the following equation [Freeze and Cherry, 1979]:

$$K_h = \frac{\sum_{i=1}^{n} K_i B_i}{B}$$
(2.1)

where, K_h is the equivalent horizontal hydraulic conductivity averaged over saturated aquifer thickness, *n* is the total number of layers in the unit, K_i is the hydraulic conductivity of lithologic layer *i*, B_i is the thickness of the layer *i*, *B* is the total thickness of the saturated unit. Since hydraulic conductivity depends on not only local lithologies but also the regional geological processes that produce them (e.g., sand in a lacustrine deposition environment may be less permeable than that in a glacial outwash environment), a range of three typical hydraulic conductivity values (minimum, mean, maximum) were defined for each lithological layer. One of the three values was assigned for the corresponding lithology, depending on the glacial land system that the water wells were drilled in [GWIM, 2006; State of Michigan, 2006].

2.4 RESEARCH APPROACHES

In this paper, we investigate how effectively the Michigan statewide groundwater database can be used to probabilistically model Michigan's groundwater systems. We consider three different approaches to model local groundwater flow and to delineate well capture zones, each representing a different way of conceptualizing aquifer heterogeneity.

These approaches are briefly described below:

1. Deterministic Approach: This is our baseline approach. We model large-scale heterogeneity as deterministic trends and the effects of small-scale heterogeneity are ignored. The approach involves solving the groundwater flow equation and performing reverse particle tracking to delineate well capture zone.

2. Stochastic Monte Carlo Approach: This approach builds on the deterministic approach and we model both large-scale heterogeneity as deterministic trend and small-scale heterogeneity as a random field using Monte Carlo simulation (MC).

We choose to use MC over the newer stochastic perturbation methods because of its conceptual simplicity, general applicability, and ability to fully quantify uncertainty in model output. MC involves directly generating many likely realizations of aquifer flow and particle tracking models in such a manner that they reflect the observed parameter uncertainty. The results are subsequently analyzed in a statistical manner to quantify the uncertainty inherent in the expected result. Combining with Michigan's statewide databases, MC represents a general and potentially very powerful tool for risk-based groundwater investigations.

3. Stochastic Macrodispersion Approach: This approach aims at significantly reducing the computational cost in practical implementation of stochastic capture zone models. The approach involves modeling groundwater flow and performing random-walk based reverse particle tracking to delineate well capture zones. Random-walk based particle tracking allows incorporating the effect of macrodispersion.

The longitudinal macrodispersivity is estimated from the following equation [Gelhar and Axness, 1983; Gelhar et al., 1992]:

$$A_L = \sigma_{lnK}^2 \lambda \tag{2.2}$$

where λ is the scale of small-scale variability and obtained from the variaogram of fluctuation of log hydraulic conductivity, σ_{lnK}^2 represents the variance of small-scale heterogeneity in log hydraulic conductivity. Transverse dispersivity is assumed to be one third of the longitudinal dispersivity [EPA, 1986].

The macrodispersion approach was originally developed for the forward solution of solute transport equation in the presence of random, small-scale heterogeneity. We extend the approach to model capture zone "macrodispersion" due to random, small-scale heterogeneity in hydraulic conductivity. We are interested in testing if macrodispersion approach can approximately reproduce the ensemble of likely capture zone realizations from Monte Carlo simulation.

For all three modeling approaches, we begin with regional scale flow modeling. A regional scale model simulates large-scale processes controlled by major streams, lakes, complex topographies and stratigraphies and provides boundary conditions for local scale models.

These three approaches discussed above are summarized graphically in Figure 2.1



Figure 2.1: Approaches used to delineate well capture zones

2.5 APPLICATION EXAMPLES

In this section, we test the utility of the statewide database and modeling system to determine probabilistic well capture zone through a systematic case study of three real sites. Our sites are selected based on data availability, data resolution, and complexity.

Figure 2.2 presents a map showing the sites, key hydrological features, pumping wells to be delineated, data distributions from water well records.

We investigate the following questions in this evaluation:

- 1. How useful is the statewide database for practical stochastic groundwater modeling?
- 2. Can the relatively crude statewide conductivity dataset be used to characterize aquifer heterogeneity with sufficient details to enable probabilistic wellhead delineation?
- 3. Can we quantify the data uncertainty? How can we separate natural variability from data noise?
- 4. How can the different database components [e.g., DEM, National Hydrological Datasets (NHDs), glacial and bedrock geology, and water well records) be combined to enable modeling stochastically complex groundwater systems?

Our systematic evaluation proceeds through the following 4 steps:

- 1. Characterization of heterogeneity at regional and local scales,
- 2. Regional scale and local scale deterministic flow modeling,
- 3. Capture zone modeling at local scale using reverse particle tracking, and
- 4. Systematic comparative analysis.

Site 1- County: Van Buren, City: Mattawan

Site 3- County: Washtenaw, City: Saline



0 8,000 16,000

m

Figure 2.2: Sites located in Michigan showing GIS features such as wells, streams, lakes, city, Type 1 wells and underground storage tanks(UST) (Site1-County:VanBuren, City: Mattawan; Site2- County-Van Buren, City: Lawton; Site3- County: Washtenaw, City: Saline)

2.6 RESULTS AND DISCUSSION

This section begins with the discussion of geostatistical site characterization using variogram modeling, at regional and local scales, followed by discussion of deterministic flow modeling at regional and local scale. Finally capture zone modeling at local scale using deterministic approach, stochastic Monte Carlo approach and stochastic macrodispersion approach are discussed and compared.

Characterization of Heterogeneity

Figure 2.3 presents variogram modeling at regional scale for log hydraulic conductivity. Figure 2.4 shows variogram modeling for the detrended log hydraulic conductivity. Table 2.1 presents a summary of the parameters of regional and local variogram models.

	Site 1	Site 2	Site3		
Variogram Information For Log Hydraulic Conductivity (Large-scale)					
Theoretical Model	Gaussian	Exponential	Exponential		
Nugget	0.26	0.3	0.8		
Range (m)	3581	6185	5796		
Resolved variability	0.14	0.14	1.2		
Variogram Information For Log Hydraulic Conductivity Fluctuation (Small-scale)					
Theoretical Model	Exponential	Exponential	Exponential		
Nugget	0.11	0.17	0.43		
Range (m)	120	120	229		
Resolved variability	0.17	0.16	0.56		

Table 2.1: Geostatistical Parameters for three sites



Figure 2.3: Variogram modeling at regional scale for log hydraulic conductivity for three sites



Figure 2.4: Variogram modeling for detrended log hydraulic conductivity for three sites

The results and our experience gained through the modeling process show:

- Variogram modeling process for hydraulic conductivity using data from the statewide database is much more robust (statistically more meaningful) than that based on limited measured data from a site-specific hydrogeological study.
- Despite data uncertainty, the variogram modeled show a clear "spatial structure".
- Variogram modeling allows identifying three-disparate scales of variability: uncorrelated data errors/noise, small-scale variability, and large scale variability.
- Variogram modeling at regional scale allow separating large scale variability from small scale variability and uncorrelated data errors.
- Kriging based on the large-scale variogram, with small scale variability and data noises represented as nuggets, can be used to delineate large scale trends. The large scale variability for the three sites has a characteristic length scale on the order of 3000m, reflecting variability associated with different glacial land systems.
- The large-scale variation from regional Kriging can be used to detrend hydraulic conductivity data.
- The residual variograms are significantly noisier than the regional variogram, but statistically meaningful structures can be detected.
- Variogram modeling of detrended log conductivity data allow identifying/ quantifying smaller spatial variability, and uncorrelated data noise.
- Variances identified for natural variability in the local models are between 0.17 and 0.52. This is relatively low because hydraulic conductivity analyzed is depth averaged. Much of the vertical variability is already averaged out.

- The small scale heterogeneities identified for the three sites have a scale on the order of 100 to 200m.
- Data noise or nugget at local scale is high, accounting for up to 40-50% of the total data variability.
- The high nugget represents data noise caused by location uncertainty associated with approximate address matching, lithologic description uncertainty, well depth variability, and reporting errors.
- Uncertainty in the assumed typical values is another important source of uncertainty and is not modeled in this study;
- DNRE's new, web-based water well data collection system with GPS-based input, realtime quality control and validation check, should significantly improve our practical ability to characterize aquifer heterogeneity in the future.

Figure 2.5 shows the kriging of conductivity distribution at regional scale and Figure 2.6 shows a realization of large-scale and detrended log conductivity at local scale.



Figure 2.5: Kriged hydraulic conductivity at regional scale. The outer boundary is the extent of regional model and inner boundary is the location of local model.



Figure 2.5 (cont'd).



Figure 2.6: A realization of residual hydraulic conductivity (Bottom) and large-scale hydraulic conductivity (Top) for the local scale model area



Large-scale K

Figure 2.6 (cont'd).



Figure 2.6 (cont'd).

A few comments are in order:

- Mean conductivity at regional scale shows a spatial pattern that is much more complex than what most site-specific hydrogeological study can provide.
- For a particular site, the simulated complex pattern is a function of (or is controlled by) only a few assigned typical conductivity values (e.g., for sand, silt, clay, gravel)
- Interpolated or simulated conductivity distribution does not go through data values because of the significant data uncertainty or high nugget.
- Large scale heterogeneity in conductivity is represented as trends deterministically in the model.
- The fluctuations around the trends are represented probabilistically in the local models.

Regional and Local Deterministic Flow Modeling

Figures 2.7 -2.9 show the simulated head distribution from the regional and local flow models for different sites. Figures 2.10 show a comparison of simulated head and static water levels from water wells in the regional model.

Table 2.1 shows key inputs and numerical parameters used in local and regional scale models. The regional scale models are simulated deterministically using no flow boundary conditions. The grid sizes and other input parameters are listed in Table 2.2.

	Site1	Site2	Site3
Boundary Condition of Regional Model	No flow	No flow	No flow
Grid Design of Regional Model (Nx, Ny)	359,287	350,254	328,330
Boundary Condition of Local model	Prescribed	Prescribed	Prescribed
Boundary Condition of Local model	Head	Head	Head
Grid Design of Local Model (Nx, Ny)	233,181	343,253	262,256
Effective Porosity	0.15	0.15	0.15
Leakance (1/day) for first, second, third,	1 2 5 10	1 2 5 10	1 2 5 10
fourth order streams	1,2,3,10	1,2,5,10	1,2,5,10
No. of Pumping Wells	2	2	2
Pumping Capacity (GPM)	700,400	950, 750	700,525
No. of particles released in each well	2000	2000	2000
fourth order streams No. of Pumping Wells Pumping Capacity (GPM) No. of particles released in each well	1,2,5,10 2 700,400 2000	1,2,5,10 2 950, 750 2000	1,2,5,10 2 700,525 2000

Table 2.2: Parameters definitions for three sites

The results and our experience gained in the modeling process shows:

- Hierarchical modeling provides a systematic framework to incorporate large scale processes in local scale modeling and to allow making maximum use of data available at different spatial scales.
- Data intensive modeling allows capturing dominant large scale groundwater processes largely controlled by surface water systems, topographies, and natural recharge. The high resolution DEM and NHDs and other derived GIS layers (e.g., estimated recharge) significantly improve our practical ability to model complex groundwater systems.

- Even without calibration, simulated heads from data intensive modeling often compares very well with observed static water levels from water well records, especially in areas glacial layer is not too thick.
- The significant spread in the model-data comparison does not mean that the simulated heads are not accurate but that data being compared to is noisy. The spread is the result of significant data uncertainty reflecting temporal variability, vertical variability, location errors, and "driller variability". Comparison between the model and static water levels from water well records must be interpreted with care.



Figure 2.7: Site1: Head field for regional model (bottom) and local model (top)


Figure 2.8: Site2: Head field for regional model (bottom) and local model (top)



Figure 2.9: Site3: Head field for regional model (bottom) and local model (top)



Figure 2.10: Comparison of predicted head and observed head (Static water level) for three sites from water wells in the regional model. Dots: Static water level from well data, Triangles: Mean static water level from well data



Figure 2.10 (cont'd).



Observed Head (m)

Figure 2.10 (cont'd).

Capture Zone Modeling:

Finally, Figures 2.11- 2.13 show well capture zone delineation by 3 different methods – the deterministic, stochastic Monte Carlo and stochastic macrodisperion.

Deterministic method results a single envelope for the extent of capture zones. The capture zone boundary is aligned with mean flow. For the sites simulated, the predicted capture zone is relatively narrow because of low pumping and strong regional flow. Unmodeled small scale processes can potentially causes significant errors in the capture zone distribution.

The stochastic macrodispersion approach is similar to the deterministic, resulting in a single envelope for the simulated capture zone. But the approach allows modeling the dispersive effects of small-scale heterogeneity.

It is interesting to notice that capture zone from stochastic macrodispersion modeling is noticeably larger than zone of uncertainty from deterministic modeling. The extent of the capture zone is lengthier, wider, and more conservative. The difference between the deterministic and macrodispersion-based delineation is the direct result of unmodeled small-scale processes and is controlled by the spatial correlation structure (scale, variance, and nugget) of the detrended hydraulic conductivity.





(b)Stochastic Monte Carlo Approach (Grey colors show probabilities of 10 (b)Stochastic Macrodispersion Approach (Grey color shows 10 years capture zone)



Legend

- Type 1 Wells
- Wells
- Underground Storage Tanks
- \Box City



Figure 2.11: Site 1: 10 years capture zone from three approaches.



Figure 2.12: Site 2: 10 years capture zone from three approaches.

(a) Deterministic Approach(Grey color shows 10 years capture zone)



(b)Stochastic Monte Carlo Approach (Grey colors show probabilities of 10 years ensemble capture zone)

2,000 4,000 m

0

(b)Stochastic Macrodispersion Approach (Grey color shows 10 years capture zone)





- Type 1 Wells
- Wells
- Underground Storage Tanks

□ City

Probability (%)



Figure 2.13: Site 3: 10 years capture zone from three approaches.

Although macrodispersion concept is widely applied in the forward modeling of contaminant transport in heterogeneous media, we are not aware of any application in the context of probabilistic wellhead protection area modeling.

Stochastic Monte Carlo gives an ensemble of capture zones. Simulation of a large number of likely capture zone realizations allows computing the likelihood of being captured for a water particle in a discrete modeling cell. The occurrence of a certain location to fall in the capture zone is presented by probability map. In Figure 2.11-2.13, dark grey color represents the area that will "certainly" be captured in 10 years, despite data uncertainty. The light grey color represents the area that is unlikely to be captured with a probability of less than 20%. The other colors represent areas that may be captured, with different levels of probability. We can clearly see how uncertainty in hydraulic conductivity results in uncertainty in the boundaries of the capture zone.

Stochastic modeling with its view of complex natural processes as spatial random variables is an ideal basis to build a risk assessment approach. Such an approach enables the concept of risk to be based on the principles of uncertainty that relate to the variability of the media. Thus uncertainty as to whether a point lies within the true capture zone can be estimated. Planning and protection considerations can be implemented according to the level of probability that a particular location lies within a capture zone in combination with the associated risk of the site polluting the aquifer. Stochastic modeling therefore represents a more reasonable solution for protecting groundwater supplies and ensuring sustainable future resources.

Limitations and Future Work

This case study has also identified a number of limitations in the database and modeling system. The most significant relevant to stochastic modeling are:

- The stochastic models presented are two dimensional. Aquifer heterogeneity delineated is depth averaged. Future research should focus on delineation of 3D heterogeneity and 3D stochastic modeling, taking advantage of the highly valuable, high resolution 3D lithologies available in the rapidly expanding water well database.
- The statewide conductivity dataset was derived based on assumed typical values for each lithologic facies. These typical values can be uncertain. Future research should consider calibrating these typical values to observed static water levels.

2.7 SUMMARY AND CONCLUSIONS

The incomplete knowledge of essential parameters and limited data availability results uncertainty in the prediction of well capture zones. In particular, the location of data points is often restricted to specific regions within the aquifer due to economic and logistic reasons. Furthermore, experimental data are always corrupted to some degree by measurement and by interpretive errors. Consequently, the location of the protection zones can only be defined in statistical manner and should therefore be represented using a probabilistic capture zone map.

In this study, we have demonstrated the usefulness of the Michigan statewide groundwater database in stochastic simulation of well capture zones. We have compared results of capture zone delineation using the traditional deterministic method, macrodispersion method, Monte Carlo simulation method.

The following findings emerge from this research:

- A significant portion of the variability in the statewide conductivity dataset is uncorrelated noise and this data noise can be quantified through variogram modeling.
- Despite the data noise, two scales of natural variability in conductivity can be identified;
- Kriging based on the large-scale variograms, with small scale variability and data noises represented as nuggets, can be used to delineate large scale trends.
- Variogram modeling of detrended conductivity data can be used to identify smaller scale heterogeneity. The residual variograms are significantly noisier, but statistically meaningful structures can be detected;
- Deterministic delineation that accounts only for the effect of large scale trend leads to capture zones that are significantly smaller than its stochastic counterpart, especially in areas where regional gradient is relatively strong;
- Stochastic Monte Carlo simulation provides a map of well capture probability. Combined with the statewide database, MC provides a useful, systematic tool for risk-based decision making;
- Stochastic macrodispersion method provides a computationally efficient alternative to delineate wellhead protection area in a way that accounts for the effect of both small and large scale heterogeneity.

Future research should focus on 3D stochastic modeling using 3D lithology and calibrating the conductivity to statewide static water level dataset.

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