Improvements in groundwater flow modeling through the integration of resistivity logs and hydraulic conductivity and the use of variogram uncertainty

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IMPROVEMENTS IN GROUNDWATER FLOW MODELING THROUGH THE INTEGRATION OF RESISTIVITY Logs AND HYDRAULIC CONDUCTIVITY AND THE USE OF VARIOGRAM UNCERTAINTY

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College
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by

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ABSTRACT

This study developed a coregionalized model to estimate hydraulic conductivity using spatial cross correlation between hydraulic conductivity and borehole geophysical data (a transform of the formation factor). An experimental pseudocross variogram is used instead of a cross variogram because data are not collocated. Experimental variogram uncertainty is investigated using confidence intervals for the experimental variogram calculated assuming variogram sills are lognormally distributed. These intervals are used for sensitivity modeling using kriging, cokriging, simulation and cosimulation.

The hydraulic conductivity fields generated by kriging, cokriging, simulation, and cosimulation are then used in a high-resolution groundwater model created using telescopic mesh refinement (TMR) from a regional flow model of the Chicot Aquifer system in southwestern Louisiana. Results are analyzed to assess the significance of adding additional information (i.e., transform of formation factor), the process (i.e., kriging versus simulation and cokriging versus cosimulation) and variogram uncertainty on the groundwater flow model. Spatial images and flow predictions using regionalized models based on sparse conductivity data only are compared with coregionalized models using both conductivity and resistivity data, and the effects on model accuracy and robustness are discussed. Coregionalized model (i.e., cokriging) and simulation process (i.e., cosimulation) significantly affect groundwater flow model prediction.

A new approach examines sensitivity of a capture zone groundwater model for the Chicot aquifer parameter uncertainty. Sensitivities to spatial variability of hydraulic conductivity, porosity, and aquifer thickness were investigated. The method calibrated aquifer properties to flow and geophysical data using cosimulation of hydraulic conductivity
and formation factor, simulation for porosity, and kriging for aquifer thickness. Geostatistical model uncertainty was analyzed with a Bayesian method. Aquifer property models were scored using integral range to preserve correlation among variogram parameters. Variogram and pseudocrossvariogram models were selected from a lower bound, median, and upper bound of the posterior probability distribution of integral range.

A steady-state two-dimensional groundwater flow model of the Chicot aquifer beneath Acadia Parish in Southwestern Louisiana examined capture zone sensitivity to spatial structure of aquifer properties. The capture zone model was insensitive to porosity variability and sensitive to hydraulic conductivity and aquifer thickness. The proposed method demonstrates the importance of model uncertainty compared with fluctuations of a fixed geostatistical model.
CHAPTER 1
STATEMENT OF THE PROBLEM

Groundwater management problems include such scenarios as design of well fields, dewatering due to a high capacity well, maintenance and sustainability of minimum and maximum water demands, and remediation of contaminated aquifers. A groundwater model can guide solutions for many of these management questions. Groundwater models require development of a conceptual model, estimation of the spatial distribution of aquifer properties, and time dependent input and output stresses. Commonly, spatial parameters of a model must be determined from limited data. Therefore, the uncertainty in these model parameters can impact management decisions. One of the major components of a successful groundwater resource management scheme is to evaluate errors in model prediction caused by parameter uncertainty.

Many studies describe and highlight the importance of incorporating model uncertainty due to parameter uncertainty in groundwater management issues. Aguado et al. [1977] present a sensitivity study analyzing the effect of hydraulic conductivity, boundary conditions, and numerical discretization schemes on dewatering strategies. The study showed conductivity changes at nodes near or at the aquifer boundary are most sensitive to drawdown. Tung [1986] used a Monte Carlo based stochastic groundwater model to study the effect of transmissivities and storage coefficients on well drawdown, demonstrating that the drawdown decreases as the coefficient of variation of transmissivity increases. Massmann and Freeze [1987a, b] performed a risk-cost-benefit analysis of waste management facilities and found that higher mean conductivity values resulted in higher failure probabilities and therefore, higher risk.
As a result of these and other works, it can be concluded that the prediction of groundwater management models are influenced by aquifer properties. Effects of uncertainty in spatial structure on flow model predictions have not been studied thoroughly. Wagner and Gorelick [1987], Morgan et al. [1993], and Chan [1994] used multiple-realizations to investigate for parameter uncertainty. Guadagnini and Franzetti [1999], van Leeuwen et al. [1998, 2000], Cole and Silliman [2000] used Monte Carlo methods to estimate uncertainty by randomly varying model properties using probability density functions. The Monte Carlo method of high-resolution models may be infeasible because these models are expensive. Feyen et al. [2002, 2003.a, 2003.b] used a Bayesian approach to stochastically analyze well capture zone with noninformative priors for the mean and covariance of transmissivity.

The goal of this dissertation research is to improve parameter estimates, quantify the parameter uncertainty using standard and newly developed geostatistical techniques, and to analyze the effect of these uncertainties on groundwater flow models using field data. In general, the study applies two stochastic approaches to groundwater management problems. First, secondary noncollocated geophysical data is used to improve hydraulic conductivity estimates; uncertainty in spatial structure and its impact on management strategy is quantified. Second, a Bayesian formulation of parameter uncertainty uses simulated variograms and studies the sensitivity of capture zone model prediction.

The organization of this dissertation study is as follows. Chapter one presents an introduction. A literature review of geostatistical methods is presented in chapter two. Aquifer hydrogeology and data used in geostatistical models are presented and discussed
in chapter three. Hypotheses and objectives of this study are discussed in chapter four. The flow model study and Capture zone modeling study are described with methods, results and discussions in chapter five and chapter six respectively. Finally, chapter seven includes conclusions and recommendations.
CHAPTER 2
GEOSTATISTICAL SPATIAL PREDICTION

Groundwater modelers often face estimation problems as data are typically available at a limited number of irregularly spaced points. Geostatistical techniques estimate aquifer properties from observed data using spatially correlated models. The techniques can estimate aquifer properties, analyze uncertainty and sensitivity in the model properties [Cressie, 1991; Goovaerts, 1997; Deutsch and Journel, 1998], and aid solution of inverse problems [e.g., Tsai and Yeh, 2004]. Geostatistics uses variograms or related techniques to quantify and model the spatial correlation structure.

Kriging

Matheron first proposed a concept of regionalized variable in regression framework and called "kriging", named after D. G. Krige, a South African mining engineer [Matheron, 1963]. The method uses the spatial covariance structure to predict a variable at new locations based on its neighbors. In regression models, least squares are used to obtain predictions where errors in estimates are assumed errors are independent. However, for some spatial properties these errors are often found to be correlated depending upon distance. In geostatistics, the dependence in errors can be incorporated through a covariance matrix $C$. The covariance matrix gives the spatial covariance, $C_{i,j}$, of a point located at position $(i, j)$. The covariance matrix is estimated by using a reasonable covariance or variogram model. The new observations in kriging, $K_{kr}(x, y, z)$, are estimated based on a weighted sum of squares of known values at existing points,
\[ \hat{K}(x, y, z) = \sum_{i=1}^{n} w_i K(x_i, y_i, z_i) \]  

(3.1)

where, \( \sum_{i=1}^{n} w_i = 1 \) for unbiased estimates and \( n \) is the number of observations.

The weights, \( w_i \), are estimated by minimizing the difference between the predicted value and the true value. Minimization of a function of \( n \) observations leads to a set of partial differential equations involving the covariance structure.

**Cokriging**

In geostatistical data, there may be additional variable(s) that are spatially correlated. The secondary variable may be observed at the same or different locations as the primary variable and such a variable may also be correlated with the primary variable. It is called collocated if both are found at the same spatial locations. It is possible that the secondary variable is more available or less expensive to obtain than the primary variable. In cokriging, the additional spatial correlation information involving the secondary variable and its cross-correlation with the primary variable is used to improve predictions. As in kriging, ordinary cokriging is used to predict unsampled locations as the weighted sum of the existing observations of primary, \( K_s(x_i, y_i, z_i) \), and secondary, \( K_F(x_j, y_j, z_j) \) variables [Goovaerts, 1997] where \( \hat{K} = \lambda_d K_d + \lambda_{2j} K_{FD} \).

\[ \hat{K}_{CK}(x, y, z) = \sum_{i=1}^{n} \lambda_{ij} K_s(x_i, y_i, z_i) + \sum_{j=1}^{m} \lambda_{2j} K_F(x_j, y_j, z_j) \]  

(3.2)

where, \( \lambda \) are weights, \( \sum_{i=1}^{n} \lambda_{ij} = 1 \) and \( \sum_{j=1}^{m} \lambda_{2j} = 0 \) for unbiased estimates and \( \hat{K} = \hat{K}_{CK}(x, y, z); \ K_d = K_s(x_i, y_i, z_i); \ K_{FD} = K_F(x_j, y_j, z_j) \). Use of covariance and
cross covariance models leads to a set of partial differential equations. Solution of the equations provides weights for the cokriging predictions. Aboufirassi and Mariono [1984] used cokriging to predict a transmissivity field using specific capacity as the secondary data. Ersahin [2003] used kriging and cokriging estimates in an infiltration study. Other successful applications of cokriging can be found in Li et al. [1999] and Gloaguen et al. [2001].

**Stationarity**

Stationarity assumptions facilitate variogram fitting. In intrinsic stationarity, the difference in the spatial variable $Z$ at two different locations has a zero mean and a constant variance i.e., $E[Z(x+h) - Z(x)] = 0$ and $Var[Z(x+h) - Z(x)] = c$ where $h$ is separation distance and $c$ is a constant. Intrinsic stationarity is the minimum stationarity requirement for traditional variogram modeling [Deutsch and Journel, 1998].

In strict stationarity, the mean and variance of the spatial variable $Z$ are assumed constant [Deutsch and Journel, 1998]. Strict stationarity also implies that the covariance between two points depends only on the difference $h$. When the empirical variogram shows an upward trend without any sign of leveling off at any distance, this indicates that the stationarity assumption is violated due to a trend or drift. In presence of strict stationarity, intrinsic stationarity is guaranteed.

**Isotropy**

Isotropy implies that the spatial dependence is a function of distance only, not direction. In omnidirectional variogram, pairs of points are lumped together for lags, regardless of angle.
\[ \gamma(\bar{x}) = \gamma(\bar{u} \mid \bar{x}), \text{ for any unit vector } \bar{u}. \]

Anisotropy implies that the spatial dependence is a function of distance and direction. Presence of an ancient river or channel could cause anisotropy. In anisotropic models, the range may change with direction while the sill remains constant; this is known as geometric anisotropy. When the sill changes with direction, it is known as zonal anisotropy. Anisotropy requires separate modeling for different angles or directions [Deutsch and Journel, 1998].

**Variogram**

The variogram is a plot of the variance of the difference in paired sample measurements as a function of the distance between samples. In variogram calculations, all possible sample pairs are examined and grouped into lags based on distance and direction. Variograms quantify the generally greater relation. Closer samples tend compared with samples far apart. The variogram (\( \gamma \)) is [Matheron, 1971].

\[ 2\gamma(h) = Var[Z(x + h) - Z(x)] \tag{3.3} \]

The variogram is estimated as

\[ 2\hat{\gamma}(\bar{h}) = \frac{1}{n(\bar{h})} \sum_{h} \left(Z(\bar{x} + \bar{h}) - Z(\bar{x})\right)^2 \tag{3.4} \]

where \( n(h) \) is the number of pairs of points which are \( h \) distance apart. Typically, distance intervals are created based on the inter-point distance set and variogram estimate for the lag or interval.

In some situations, there could appear to be variability at zero lag distance indicative of very short range variability. In this case, the experimental variogram does
not extrapolate to the origin; this is called the nugget effect. A constant variogram indicates no spatial dependence. This situation is known as a pure nugget effect.

For a stationary process, the sample variogram rises to an upper bound or sill equal to the variance of the spatial variable. The distance at which this occurs is the range. If no upper bound is reached in the sample variogram that indicates non-stationarity or anisotropy at the scales investigated. When the spatial pattern is difficult to interpret, subregional variograms as well as directional variograms should be considered. More data points are necessary in case of directional variograms. For a directional variogram, we must specify an azimuth tolerance i.e., the number of degrees around the directional vector. In the case of smaller dataset a large enough tolerance is necessary to get enough points at each interval.

**Variogram Modeling**

Variogram models are a functional forms of the covariance that safely two necessary mathematical conditions must be satisfied: symmetry i.e., $C(x,y) = C(y,x)$, and positive definiteness [Goovaerts, 1997]. The most common variogram models are the exponential and spherical functions that rise to a sill and within the range observations are correlated.

A variogram model can be fit to an experimental variogram interactively or by eye. A non-linear least square method can be used to find a best fit where the objective function minimizes the residual sum of squares between the theoretical and empirical variogram. Weighted non-linear least squares are also used when the number of points per lag is very different [Cressie, 1991]. In weighted least squares the weights are
calculated based on the number of points and are included in the residual function to be minimized.

**Variogram Model Parameters**

The sill is the population variance or the variance at a lag where the variable is no longer correlated. For example, the range of a spherical model is the distance at which the model reaches its maximum value (i.e., the sill). The nugget is the intercept of the variogram model representing local variation at zero lag distance possibly due to measurement error or scaling issues (Figure 2.1).

The ratio of the nugget to the sill is often referred to as the relative sill. If this fraction is high, then non-spatial variations constitutes most of the variability in the variable and a spatial model becomes less practical [Deutsch and Journel, 1998].

![Figure 2.1: Diagram showing variogram parameters](image)

**Integral Range**

The integral range quantifies statistical fluctuations and correlations of a stochastic model [Lantuejoul, 2002]. The integral range is the area under the correlogram curve.
\[ R_I = \int_0^\infty \rho(h)dh \]

where \( \rho \) is the correlogram and \( h \) is the separation distance. We can rearrange it to get

\[ R_I = \int_0^\infty \rho(h)dh = \int_0^\infty \frac{C(h)}{S}dh = \int_0^\infty \frac{S - \gamma(h)}{S}dh = \int_0^\infty \left(1 - \frac{\gamma(h)}{S}\right)dh \tag{3.5} \]

where, \( C(h) \) is the covariance, \( \gamma(h) \) is the semivariogram, and \( S \) is the sill. As \( \frac{\gamma(h)}{S} = 1 \) for the distance greater than the range, the above equation is equivalent to

\[ R_I = \int_0^\infty \left(1 - \frac{\gamma(h)}{S}\right)dh . \]

**Variogram Uncertainty**

The variance of a variogram characterizes uncertainty in the variogram model as parameters cannot be precisely estimated from available data. Ortiz and Deutsch [2002] describe a theoretical approach to calculate pointwise variance estimates for each lag. Using the variogram variance we can generate extreme scenarios assuming a probability distribution.

**Regionalized and Coregionalized**

In a regionalized model only one variable is analyzed. In a coregionalized model, multiple variables are analyzed separately to determine the contribution made by each variable to an observed result [Goovaerts, 1997]. Coregionalized models exploit correlation between the mean of one variable to another. Kriging and simulation are regionalized models and cokriging and cosimulation are coregionalized models.
Types of Kriging

In **simple kriging**, the mean of the region is assumed to be known and constant. However, this is not true in most cases [Deutsch and Journel, 1998].

In **ordinary kriging**, the unknown mean is estimated but assumed constant. In the ordinary kriging equations, the system of linear equations includes a constraint equation for the weights summing to 1. Ordinary kriging follows spatial covariance modeling and is a prediction method that requires, at a minimum, an intrinsic stationary assumption (i.e., mean difference=0) [Deutsch and Journel, 1998].

In **universal kriging**, other variables could be used to estimate the mean. For example, the mean may vary with geographic coordinates (x, y) and depend on covariates at other locations. The additional predictors are typically physical/environmental characteristics taken at each location. In universal kriging one has to estimate the mean and covariance structure together [Deutsch and Journel, 1998].

In **local kriging**, a pre-defined neighborhood distance cuts off the possible points in the kriging system and all prediction is done within this neighborhood. In this way the constant mean assumption is only required within the neighborhood [Deutsch and Journel, 1998].

In **block kriging**, a block estimate of a variable gives an average over a subregion. It is algebraically equivalent to an average of the ordinary kriging estimates [Deutsch and Journel, 1998].
Simulation

Simulation techniques simulate the kriging error as a correlated random process. The kriging estimation error is \( [z(x) - \hat{z}(x)] \) for any \( x \notin \) measured data, where \( z(x) \) is unknown. Because simulation adds back the estimation error, the variance in the model (co)variograms is preserved. Simulation is relevant for groundwater flow models as high and low values may control flow behavior [Fogg, 1986]. The average of many possible realizations is equal to the kriging value at the same location [Deutsch and Journel, 1998]. **Conditional simulation** generates values that have specified mean and covariance and reproduces observed data at data locations [Deutsch and Journel, 1998].
CHAPTER 3
DATA ANALYSIS

Hydrogeology of the Chicot Aquifer

The Chicot system is the principal source of groundwater for southwestern Louisiana and is the most heavily pumped aquifer in the state. Rice irrigation accounts for nearly 90% of the groundwater pumped from the aquifer [Sargent, 2002]. A number of studies of this aquifer system established the hydrogeologic framework of this study.

Geology

The Chicot aquifer system consists of a complex series of alternating beds of unconsolidated sand, gravel, silt, and clay [Nyman, 1984]. Investigators have divided the Chicot aquifer system differently. Nyman [1984] has divided the aquifer into four regions: the Lake Charles area, the rice growing area, the outcrop area, and the Atchafalaya river basin. Jones [1950] further subdivided the Chicot aquifer system in the Lake Charles industrial area into three major aquifers: the 200 feet sand, 500 foot sand, and 700 feet sand. The names were based on average depths of wells completed in these aquifers.

The Chicot aquifer consists of thick sand and gravel deposits that dip and thicken southward from southern Vermilion and Rapides parishes. The aquifer thins to the west and continues into Texas. The aquifer thickens to the east toward the axis of Mississippi Embayment. The aquifer units thicken gulfward but are subdivided by clays [Nyman, 1984]. The confining clay of the Chicot aquifer system generally thickens consistently from the outcrop in the north to the coastline, ranging from 1 – 500 feet thick. The clay beds consist primarily of mixed layer clay and smectites. Ancient rivers in the eastern part of the study area had smaller drainage areas and flow rates than the ancestral Mississippi river. The
eastern deposits therefore consist of thinner, finer grained beds separated by thick clay [Nyman, 1984].

The Chicot aquifer system underlying Acadia parish comprises alternating beds of consolidated sand, gravel, silt and clay [Carlson, 2003; Figure 3.1(a)]. This part of the Chicot is divided into two aquifer units: the upper and lower aquifers [Carlson, 2003] that are separated by clay lenses referred to as the Upper/Lower confining zone [Nyman et al., 1990]. The upper Chicot is as much as 200 feet thick the study area and contains mostly coarse sand grading to gravel basal beds. The upper and lower aquifers generally are several hundred feet thick and are separated in places by thin clays.

Hydrology

The recharge area of Chicot aquifer system in Louisiana is in the southern Vermilion and Rapid parishes and in northern Beauregard, Allen, and Evangeline parishes [Nyman et al., 1990]. Under predevelopment conditions (pre-1900), the ground water flow was primarily from recharge areas southward toward the coast and eastward in the Atchafalaya river basin. As a result of industrial and agricultural development, flow throughout the aquifer system now converges to the pumping centers in the rice growing area and Lake Charles area [Nyman et al., 1990]. Under 1981 conditions, vertical leakage was the largest component of the recharge and water driven from aquifer storage is a relatively small part of flow in the aquifer system [Nyman et al., 1990]. The primary impact on the ground water flow system in the Chicot aquifer is due to the increased acreage of rice planting.

Water Quality

Fresh water in Chicot aquifer system is calcium bicarbonate type. Ground water from this aquifer system generally is suitable for irrigation and industrial use, but contains locally
high iron concentrations (greater than 0.3 mg/l) and requires treatment for public supply use [Moody et. al., 1986]. 653 samples of water from the Chicot aquifer indicate hardness ranges from 3 –700 mg/l and averages about 130 mg/l [Tomasczeski, 1992].

**Hydrogeologic Data**

This study uses hydrogeologic data from the portion of Chicot aquifer underneath Acadia parish. The dataset includes hydraulic conductivity values and resistivity logs [figure 3.2]. The resistivity logs [figure 3.1(b)] are used to derive a transformed formation factor and to determine the porosity and aquifer thickness at the well locations.

**Hydraulic Conductivity Data**

Hydraulic conductivity measured how well water will flow through a substance. Accurate hydraulic conductivity values are crucial in a groundwater flow model. The hydraulic conductivity values used in this study were calculated from pumping tests using a semi-empirical method [Bradbury and Rothschild, 1985; Carlson et. al., 2003]. For the Acadia parish study, 42 tests are available. The specific capacity tests were analyzed using the following equations.

\[
T = \frac{Q}{4\pi(s - s_w)} \left[ \ln \left( \frac{2.25Tt}{r_w^2S} \right) + 2s_p \right]
\]

(3.1)

where,

\[
s_w = CQ^2
\]

(3.2)

\[
s = \frac{Q}{4\pi T} \left[ \ln \left( \frac{2.25Tt}{r_w^2S} \right) + 2s_p \right]
\]

(3.3)

\[
s_p = \frac{1 - \frac{L}{b}}{\frac{L}{b}} \ln \left( \frac{b}{r_w} - G\left( \frac{L}{b} \right) \right)
\]

(3.4)

\[
G(\cdot) = \frac{1}{2} \ln \left( \frac{1 + \sqrt{1 - 4\pi(\cdot)}}{1 - \sqrt{1 - 4\pi(\cdot)}} \right)
\]

(3.5)
where, $b$ is aquifer thickness, $L$ is length of screen interval, $G$ is a function of the ratio of $L/b$, $s_w$ is well loss, $C$ is well loss constant, $Q$ is discharge, $s_p$ is partial penetration factor given by equation 3.4, $r_w$ is radius of well, $S$ is storage coefficient, $t$ is pumping time $s$ is drawdown in the well, and $T$ is transmissivity.

During a specific capacity test, drawdown($s$) versus time ($t$) is measured while the well pumping rate is held constant. The technique solves equation 3.1 in iteratively with taking equations 3.2, 3.3, 3.4, and 3.5 as an input to equation 3.1. Hydraulic conductivity ($K$) was determined by dividing the transmissivity by the aquifer’s sand thickness. Sand thicknesses were determined by analyzing well log data.

**Resistivity Data**

Secondary data can be used to improve spatial models of the hydraulic conductivity. Fifty-three resistivity values were estimated from resistivity logs obtained from wells located in the study area [figure 3.2]. The oil and gas geophysical resistivity logs were obtained from the Louisiana Department of Natural Resources, Office of Conservation (OC) Well Log Library.

The formation factor of a sand aquifer is defined as

$$F = \frac{R_a}{R_w} \quad (3.6)$$

where, $F =$ Formation resistivity factor, $R_a =$ Saturated formation resistivity, and $R_w =$ Formation water resistivity [Archie, 1942]. The logs [e.g., figure 3.1(b)] were divided into 3.05 m (10 ft) sections between the top and bottom elevation of the upper
Figure 3.1: (a) Cross section G-G’ through southern Acadia parish, (b) Geophysical log illustrating the various horizons in the Chicot Aquifer, Acadia Parish, Louisiana (Well# 078272, Hickman#1, Sec 3 T10S R1E) (after Hanson et al., 2001) (from Mathematical Geology, with permission)
Figure 3.2: (a) Study area (b) Chicot Aquifer regional model grid (c) Acadia parish model grid with location of hydraulic conductivity dataset and resistivity logs that are used to calculate transformed formation factor, porosity and thickness of aquifer (from Mathematical Geology, with permission).
The formation factor of a sand aquifer is defined as

\[ F = \frac{R_o}{R_w} \]  

(3.6)

where, \( F \) = Formation resistivity factor, \( R_o \) = Saturated formation resistivity, and \( R_w \) = Formation water resistivity [Archie, 1942]. The logs [e.g., figure 3.1(b)] were divided into 3.05 m (10 ft) sections between the top and bottom elevation of the upper Chicot aquifer. The maximum resistivity reading for each section was taken as \( R_o \) for the corresponding section. The formation water resistivity was assumed constant, which is reasonable at the scale of this study. Because the water characteristics are assumed constant, any variance in the sand formation resistivity factor reflects differences in particle size and tortuosity. Thus, the formation factor is proportional to the formation resistivity. The effective formation factor over the depth of the upper Chicot was calculated as the average of the formation factors calculated for all 3.05 m (10 ft) sections within the unit.

Formation factor can be related to the porosity by the Archie equation [1942]:

\[ F = \frac{a}{\Phi^m}, \text{ or} \]

\[ \Phi = \left( \frac{a}{F} \right)^{\frac{1}{m}} \]  

(3.7)

where, \( a \) = pore geometry coefficient, \( \Phi \) = porosity as a decimal fraction, and \( m \) = cementation factor. The hydraulic conductivity can be calculated from the Kozeny-Carmen equation [Carmen, 1956]:

\[ \frac{1}{K} = \frac{C \Phi^2}{\Phi(1-\Phi)} \]  

where, \( K \) = hydraulic conductivity, \( C \) = Kozeny constant.
\[ K = \frac{\rho g}{\mu} \frac{\Phi^3}{(1 - \Phi)^2} \frac{d_m^2}{180} \]  

(3.8)

where, \( d_m \) = mean particle diameter, \( \Phi \) = Effective porosity. \( \rho \) = fluid density, \( g \) = gravitational force and \( \mu \) = fluid viscosity. Substituting equation (3.7) into (3.8) gives the hydraulic conductivity based on the formation factor.

\[ K_F = \frac{\rho g}{\mu} \frac{1}{F^{m_k} a^{m_k}} \frac{3}{d_m^2} \frac{1}{180} \]  

(3.9)

In this work, \( K_F \) is used as a secondary variable that is linearly related to hydraulic conductivity. To maximize linear correlation, the constant is irrelevant. Thus, the secondary variable is defined as

\[ f = \frac{1}{F^{m_k} a^{m_k}} \frac{3}{d_m^2} \frac{1}{180} \]  

(3.10)

For the portion of the Chicot aquifer underlying Acadia parish, the average particle diameter is \( d_m = 0.43 \) mm (1.22 in phi units; USGS unpublished data files). Typically, values of \( a \) vary between 0.62 and 2.45, and values of \( m \) range between 1.08 and 2.15 depending on sediment or rock type [Asquith and Gibson, 1982]. The values for \( a \) and \( m \) in this system were determined by maximizing the short-distance covariance between hydraulic conductivity \( (K) \) and transformed formation factor \( (f) \) using nonlinear regression [Developing Microsoft Excel 95 Solutions, Microsoft Press, 1995] [figure 3.3]. For this dataset, \( \hat{a}_k = 1.76 \) and \( \hat{m}_k = 1.64 \).
Figure 3.3: Maximized short distance covariance between hydraulic conductivity \(K\) and transformed formation factor \(f\) to estimate values of \(a\) and \(m\). The zero-lag covariance is unknown because no points are collocated.

Figure 3.4: Cross plot between hydraulic conductivity \(K\) and transformed formation factor \(f\) at short distances. Both variable has normal score transformed values.
**Porosity Data**

The porosity is computed from sand resistivity from geophysical logs. Fifty-three geophysical logs are analyzed and average resistivity values for the upper Chicot section are calculated for every 10 ft interval. Porosity is calculated from formation factor using the Archie equation [Archie, 1942]. The $a$ and $m$ used for the porosity calculation are not the same as for the transformed formation factor; $a_k$ and $m_k$ are intended to maximize the linear correlation between the transformed formation factor ($K_F$) and the hydraulic conductivity. Thus, $a_k$ and $m_k$ are influenced by additional factors such as particle size and do not solely reflect porosity. Porosity was calculated using $a_\phi$ and $m_\phi$ from the Humble formula for unconsolidated sand [Asquith and Gibson, 1982]. Because the purposes of the two correlations (i.e., for transformed formation factor and porosity) are different, different $a$ and $m$ values are optimal.

**Thickness Data**

The available geophysical logs are used to determine elevations of top and bottom of upper Chicot in Acadia Perish. Elevation of top and bottom of the aquifer are selected on the resistivity curve from the points of inflection. The differences between the two elevations estimate thickness of upper Chicot. Using this procedure, 54 aquifer thicknesses are obtained within the study area.

**Data Analysis**

**Descriptive Statistics**

A traditional descriptive statistical analysis of the data is performed in order to know the summary statistic of the hydrogeological variables, hydraulic conductivity, transformed formation factor, porosity, and thickness. [Table 3.1 and figure 3.4].
Normality

Hydraulic conductivity is positively skewed as (its log is nearly symmetric) expected [figure 3.4; Domenico and Schwartz, 1990]. Therefore, they were standardized to zero mean and unit variance to account for the skewness and transformed normal distribution. The transformation is performed using the nscore program of GSLIB [Deutsch and Journel, 1997].

Stationarity

After ensuring that the transformed data are normally distributed, the next step is to examine stationarity. Stationarity is satisfied if the distribution of the variable $Z(x, y)$ is independent of location $x$ and $y$. This implies that mean and variance are the same everywhere. All variables were tested for stationarity by analyzing the $t$-statistic from a linear model. This linear model was fit in the $x$ and $y$ directions to analyze if there is any trend or if the mean varies spatially. The $t$-test statistics from analysis of variance table of linear models [Table 3.2] show that in all cases there is no significant trend in $x$ or $y$ direction at a 10% level of significance.
Figure 3.5: Histograms for aquifer properties.
Table 3.1: Summary statistics for the variables

<table>
<thead>
<tr>
<th>Minimum</th>
<th>18</th>
<th>43</th>
<th>0.30</th>
<th>52</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st Quantile</td>
<td>108</td>
<td>62</td>
<td>0.31</td>
<td>208</td>
</tr>
<tr>
<td>Median</td>
<td>203</td>
<td>74</td>
<td>0.34</td>
<td>263</td>
</tr>
<tr>
<td>Mean</td>
<td>289</td>
<td>81</td>
<td>0.35</td>
<td>256</td>
</tr>
<tr>
<td>3rd Quantile</td>
<td>282</td>
<td>92</td>
<td>0.37</td>
<td>308</td>
</tr>
<tr>
<td>Maximum</td>
<td>2297</td>
<td>418</td>
<td>0.44</td>
<td>373</td>
</tr>
<tr>
<td>Stand. Dev.</td>
<td>378</td>
<td>49</td>
<td>0.04</td>
<td>71</td>
</tr>
</tbody>
</table>

where

- $K$ is hydraulic conductivity
- $K_F$ is transformed formation factor
- $\phi$ is porosity
- $T$ is aquifer thickness

Table 3.2: t-test statistic from bilinear model fitted to the $x$- and $y$- directions to detect trends

<table>
<thead>
<tr>
<th>Variable</th>
<th>Model</th>
<th>t-test</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$X$, $Pr&gt;0.161$</td>
<td>$X$, $Pr&gt;0.052$</td>
</tr>
<tr>
<td>$K$</td>
<td>$K \approx X + Y$</td>
<td>0.943</td>
</tr>
<tr>
<td>$K_F$</td>
<td>$K_F \approx X + Y$</td>
<td>0.167</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$\phi \approx X + Y$</td>
<td>0.320</td>
</tr>
<tr>
<td>$T$</td>
<td>$T \approx X + Y$</td>
<td>0.050</td>
</tr>
</tbody>
</table>
CHAPTER 4
PROPOSED APPROACH

Groundwater flow models are used in many management and regulatory applications such as the determination of water well pumping rates, forecasting aquifer sustainability, and mapping water well capture zones. The development of a groundwater flow model requires selecting models and parameters to describe the aquifer system heterogeneity. In this dissertation, a groundwater flow model of the Chicot aquifer system in Acadia parish is being used to assess uncertainty in aquifer system responses caused by aquifer heterogeneity. A study of this particular system presents challenges that are common in groundwater modeling. First, few hydraulic conductivity data and resistivity logs, which can provide additional hydrogeological data are available. Next, the use of resistivity data is complicated as the relationship with hydraulic conductivity is nonlinear and none of the hydraulic conductivity and resistivity data is collocated. In addition, the variogram parameters are uncertain because they are inferred from limited data. Moreover, model sensitivity to some aquifer properties, geostatistical simulation methods, and uncertainty in variogram parameters are poorly understood. These considerations motivated two component of this study to address the above difficulties and provide solutions using available field data of the Chicot aquifer system.

In the first component of the dissertation work, a groundwater flow model is used to examines the impact of regionalized and coregionalized hydraulic conductivity fields, variogram uncertainty and simulation processes for an aquifer system. This study compares two regionalized models (kriging and sequential Gaussian simulation) and two coregionalized models (cokriging and cosimulation). The research assesses the significance
of the coregionalized variable, simulation processes, and variogram uncertainty on the groundwater flow system.

The second study component focuses on the sensitivity of modeling efforts on geostatistical model parameters, with the goal of increasing confidence in the capture zone model. This part of the study examines three properties (i.e., hydraulic conductivity, porosity, and aquifer thickness) and analyzes the impact of their variability on the capture zone size and shape.

**Hypotheses**

The overall goal of this research is to improve to quantitative spatial aquifer property prediction and to assess the impact of the uncertainty in these fields on groundwater flow predictions. Specifically, the hypotheses are:

1. The incorporation of additional geophysical data (i.e., a transformed hydraulic conductivity value based on the formation factor) improves our ability to generate hydraulic conductivity fields with lesser and petrophysically justified levels of uncertainty;

2. Variogram parameter uncertainty has a significant impact on groundwater modeling and capture zone delineation; and

3. The use of variogram uncertainty in determining capture zone uncertainty is an efficient and effective alternative to Monte Carlo methods.

**Objectives**

The objectives of this dissertation research are to study three aspects of groundwater modeling:
1. Improved groundwater system models and estimation of the uncertainty in the variograms used to generate the hydraulic conductivity, porosity and thickness of aquifer.

2. Assessment of the value of coregionalized models by examining uncertainty in variogram parameters and geostatistical and flow models of aquifers.

3. Formulate uncertainty estimates by correlating all variogram and crossvariogram parameters against the integral range allowing comparison of the effects of uncertainty in model properties for hydraulic conductivity, porosity, and thickness.
CHAPTER 5
GROUNDWATER FLOW MODELING

Introduction

Problem Statement and Motivation

Groundwater models are widely used to predict the availability and performance of water supplies. Numerical solutions of the partial differential equations describing groundwater flow can integrate diverse geologic, hydrologic, and engineering data [Anderson Woessner, 1992]. Theoretical [e.g., Gelhar et al., 1983] and empirical studies [e.g., Neuman, 1990; Poeter et al., 1990] demonstrate that hydraulic conductivity heterogeneity significantly affects model predictions, and careful treatment of this variability is therefore warranted.

A study of the Chicot aquifer in Acadia parish presents challenges that are common in groundwater modeling:

- Hydraulic conductivity data must be inferred from pumping tests. Standard, semi-empirical methods are used in this study.
- Few pump test data are available. For the Chicot study in Acadia parish, 42 tests are available in an area of approximately 2252 km² [figure 3.2].
- Wireline log data augment the available pump tests–53 resisitivity logs are available in the same 2252-km² area [figure 3.2]. These “secondary” data can be used to improve spatial models of the “primary” variable, hydraulic conductivity. However, use of the secondary data is complicated because the relationship with the primary variable is nonlinear, and the primary and secondary data are not be collocated in the study area.
The parameters describing the spatial variability of hydraulic conductivity and electrical resistivity are uncertain. The usefulness and interpretation of modeling results must be considered in light of this multilevel uncertainty.

These considerations drove formulation and application of coregionalized models incorporating model uncertainty for the Chicot aquifer. The elements and goals of this study are discussed first. Next, the methods to be used are discussed. Data and modeling results for the parish-scale study are then described. Finally, the results are interpreted statistically and implications for model choice and interpretation are presented.

**Estimation and Simulation of Hydraulic Conductivity**

Numerical groundwater flow models require description of aquifer system heterogeneity. Hydraulic conductivity is highly variable and uncertain, and flow and transport behavior are sensitive to conductivity [Rehfeldt et al., 1992; Neuman, 1990; Poeter et al., 1990]. Geostatistical methods such as kriging have been used to estimate hydraulic conductivity distribution from sparse data [Clifton et al., 1982]. However, simulation methods [Delhomme, 1979] better reproduce high and low hydraulic conductivity values and allow stochastic assessment of flow model uncertainty [Isaaks and Srivastava, 1989]. A number of studies have evaluated and compared various techniques for estimating hydraulic conductivity fields. Ritzi et al. [1994] compared three indicator-based geostatistical methods to predict zones of higher hydraulic conductivity. Eggelston et al. [1996] compared the hydraulic conductivity structure and its sensitivity by using two estimation methods (kriging and conditional mean) and two simulation methods (sequential Gaussian and simulated annealing) and found that simulations better reproduce local contrasts and large-scale features. Boman et al. [1995] studied the response of a transport model to four schemes
(three deterministic and one fractal-based stochastic) to interpolate field-measured hydraulic conductivity data, concluding that kriging and fractal interpolation were not significantly better than simpler methods; his study was based on densely-sampled measurements which may not be typical of groundwater studies. Varljen et al. [1991] and Lin et al. [2000] also used simulation to generate hydraulic conductivity distributions.

**Use of Secondary Data for Spatial Modeling**

If primary data are sparse and secondary variable is strongly correlated to the primary variable, coregionalized models can improve estimates of the primary variable. Aboufirassi and Mariano [1984] used cokriging to predict a transmissivity field using specific capacity as the secondary data and reported that cokriging improved estimates. Ersahin [2003] used kriging and cokriging estimates in an infiltration study and found cokriging was superior to kriging with limited primary data. Other applications of cokriging to estimate hydraulic conductivity can be found in Li et al. [1999] and Gloaguen et al. [2001]. The studies mentioned above used collocated data for the secondary variable; however, measurements may not be collocated.

**Secondary Datum: Electrical Resistivity**

The formation factor [obtained from well resistivity logs; Asquith and Gibson, 1982] is a relatively common and low cost measurement, particularly compared to pumping tests. Kelly [1977] and Kosinski and Kelly [1981] studied site-specific electrical resistivity and hydraulic conductivity and established empirical relationships between formation factor and hydraulic conductivity. However, their study did not investigate the theoretical basis for the correlation and the empirical relationship is not necessarily applicable to other sites. This
paper extends their work by transforming the geophysical resistivity data to the hydraulic conductivity by the Archie relation [1942] to estimate porosities an the Kozeny-Carman [Carman, 1956] to convert porosities to hydraulic conductivity for sand units.

**Geostatistical Model Parameter Uncertainty**

In groundwater studies, measurements of hydraulic conductivity are typically sparse. Conductivity fields estimated using regionalized models such as kriging or simulation are therefore highly uncertain, as the precision of these methods depends on data density. Eggleston et al. (1996) studied a densely sampled aquifer and reported that the number of observations significantly affects hydraulic conductivity models.

Whether one uses a regionalized or coregionalized model, the spatial structure is estimated from field observations. Data sparseness and uncertainties associated with the field measurements lead to uncertainties in the correlation model, which are commonly neglected. Kitanidis [1986] examined the effect of parameter uncertainty in a Bayesian framework. Feyen et al. [2003] examined parameter uncertainty for capture zones in a Bayesian framework, concluding that predictions of fitted models do not reflect field variance.

Variogram uncertainty is assessed for coregionalized models using a Gaussian approximation [Ortiz-C. and Deutsch, 2002]. The uncertainty estimates are used to examine the importance of alternative, plausible geostatistical models.

**Summary of Approach**

A groundwater flow model is used to examine the impact of regionalized and coregionalized hydraulic conductivity fields, variogram uncertainty, and simulation
processes on the Chicot aquifer. Two regionalized models (kriging and sequential Gaussian simulation) and two coregionalized models (cokriging and cosimulation) are compared. Analysis of variance assesses the significance of secondary data, geostatistical method, and variogram uncertainty on the groundwater flow behavior. Finally, because the secondary variable (the formation factor) is not collocated with the hydraulic conductivity data, a pseudocross variogram method [Clark et al., 1989] is used.

The data set includes 42 hydraulic conductivity and 53 formation factor measurements. A transform is inferred to maximize linear correlation between formation factor and conductivity at small separation distances; this transformed formation factor is used as the secondary variable. A pseudocross variogram is used because the primary and secondary variables are noncollocated. A weighted linear least squares method estimates the variogram and the pseudocross variogram parameters. Positive-definiteness is imposed on the linear model of crosscovariance as required [Goovaerts, 1997]. The cosimulated hydraulic conductivity fields honor a full linear model of cross covariance. The mean, 95 percent upper bound and 5 percent lower bound of correlations are estimated [Ortiz C. and Deutsch, 2002] assuming lognormal distribution in both auto- and cross-covariance (or variograms).

The effects of hydraulic conductivity heterogeneity are tested using a high-resolution local model that incorporates aquifer stratigraphy and approximately 400 water wells. The boundary conditions for this model were obtained using telescopic mesh refinement [Leake and Claar, 1999] on a regional aquifer groundwater model.
Application

The Chicot aquifer in southwest Louisiana is the most heavily pumped aquifer in the state. Rice irrigation accounts for about 85 percent of the groundwater pumped from the aquifer in Acadia parish [Sargent, 2002]. The aquifer comprises interbedded unconsolidated sand, gravel, silt and clay [Nyman et al., 1990]. In Acadia Parish, the Chicot system is divided into Upper and Lower Chicot units separated by clay lenses referred to as the Upper/Lower confining zone [figure 3.1(a); Hanson et al., 2001]. Recharge occurs primarily by the direct infiltration of rainfall and outcrop areas [Nyman et al., 1990].

A groundwater flow model assesses uncertainty in aquifer responses caused by heterogeneity. Similarly flow models have been used in many regulatory applications such as well pumping, aquifer sustainability, and capture zone analysis. Aquifer recharge and discharge must be known for aquifer regulation. The simulated drawdown from a groundwater flow model is also used to determine well specific capacity. Specific capacities reflect conductivity to water or potential to supply water from the aquifer, which affects groundwater resource management. For example, management guidelines may stipulate that the average water level for a region should not drop below specified levels.

Methods

Formation Factor

The formation factor of a sand aquifer is

\[ F = \frac{R_o}{R_w} \]

where, \( F \) = Formation resistivity factor, \( R_o \) = Saturated formation resistivity, and \( R_w \) =
Formation water resistivity [Archie, 1942]. Oil and gas geophysical resistivity logs were obtained from Louisiana Department of Natural Resources, Office of Conservation (OC) Well Log Library. The logs [e.g., figure 3.1(b)] were divided into 3.05 m (10 ft) sections between the top and bottom elevation of the upper Chicot aquifer. The maximum resistivity reading for each section was taken as $R_0$ for the corresponding section. The formation water resistivity was assumed constant, which is reasonable at the scale of this study. Because the water characteristics can be assumed to be constant in this aquifer, the variance in the sand formation resistivity factor reflects differences in particle size and tortuosity. Thus, the formation factor is proportional to the formation resistivity. The effective formation factor over the depth of the upper Chicot was calculated as the average of the formation factors calculated for all 3.05 m (10 ft) sections within the unit. The effective formation factors are transformed to porosity and porosity data are transformed to hydraulic conductivity using a form of Kozeny-Carmen equation [Carmen, 1956]. Details of the method are discussed in chapter hydrogeologic data section of chapter three.

Normality and Stationarity

The transformed formation factor data was separated into three 50 ft layers according to elevation (from 150 to 300 ft below mean sea level). $K$ and $f$ were tested for trends by analyzing the $t$-statistic from a bilinear model. This bilinear model was fit in the $x$- and $y$-directions to detect trends; there is no significant trend in $x$ or $y$ direction at a 10 percent level of significance [table 5.1]. Hydraulic conductivity and transformed formation factor are positively skewed [figure 5.1(a-d)] which is reasonable for sands that have hydraulic conductivity that is log-normally distributed [Domenico and Schwartz, 1990]. Therefore, they were standardized to zero mean and unit variance and transformed to normal scores.
The normal transformation facilitated computation of the pseudocross variogram, which requires both variables have the same mean and variance.

**Experimental Variogram and Pseudo Cross Variogram**

The 42 measurements of hydraulic conductivity and 53 values of the transformed formation factor are used in the univariate (i.e., $K$) and coregionalized (i.e., $K$ and $f$) models. The two autovariograms ($\gamma_K(h)$, and $\gamma_f(h)$) are calculated from [Matheron, 1971]:

$$\gamma_K(h) = \frac{1}{2} E \left[ (K(x+h) - K(x))^2 \right]$$  \hspace{1cm} (5.5)

where, $K(x+h)$ and $K(x)$ are measured hydraulic conductivity at coordinate $(x+h)$ and $x$ respectively; the variogram $\gamma_f(h)$ is defined analogously where $K$ is replaced by $f$.

The coregionalized model is usually developed from a cross variogram between the two variables,

$$\gamma_{KF}(h) = \frac{1}{2} E \left[ (K(x+h) - K(x))(f(x+h) - f(x)) \right]$$  \hspace{1cm} (5.6)

Because none of the data in this study area are collocated, a pseudocross variogram was used instead of usual cross variogram. Clark et al. [1989] introduced the pseudocross variogram as the expected squared difference between the random variables measured at different locations; i.e.,

$$\tilde{\gamma}_{KF}(h) = \frac{1}{2} E \left[ (K(x+h) - f(x))^2 \right]$$  \hspace{1cm} (5.7)

where $\tilde{\gamma}_{KF}$ is pseudocross variogram estimator. Experimental variograms were computed using conventional methods [Deutsch and Journel, 1998].
Variogram Model

Variogram models determine kriging weights and variance levels. These models are especially important in this study because the variogram uncertainty assessment uses a pre-defined, parametric variogram model. Spherical, exponential, and Gaussian models are commonly used to describe the variogram structure [Deutsch and Journel, 1998]. This study

Table 5.1: t-test statistic from bilinear model fitted to the \( x \)- and \( y \)- directions to detect trends

<table>
<thead>
<tr>
<th>Variable</th>
<th>Model</th>
<th>( X, Pr &gt; t )</th>
<th>( Y, Pr &gt; t )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K )</td>
<td>( K \sim X + Y )</td>
<td>0.06</td>
<td>0.82</td>
</tr>
<tr>
<td>( f_1 )</td>
<td>( f_1 \sim X + Y )</td>
<td>0.54</td>
<td>0.94</td>
</tr>
<tr>
<td>( f_2 )</td>
<td>( f_2 \sim X + Y )</td>
<td>0.67</td>
<td>0.35</td>
</tr>
<tr>
<td>( f_3 )</td>
<td>( f_3 \sim X + Y )</td>
<td>0.05</td>
<td>0.47</td>
</tr>
</tbody>
</table>

where, \( K \) = Hydraulic conductivity
\( f_1, f_2, f_3 \) = Transformed formation factor separated at 50 ft interval

Figure 5.1(a-d): Histogram plot of hydraulic conductivity and transformed formation factor. All distributions are positively skewed, motivating a data transform.
used a spherical variogram model, which shows moderate correlation at short range (as expected when investigating hydraulic conductivity). The spherical variogram model is

$$\gamma(h) = c \left\{ \frac{3h}{2a} - \frac{1}{2} \left( \frac{h}{a} \right)^3 \right\}, \quad h \leq a$$

$$\gamma(h) = c, \quad h \geq a$$  \hspace{1cm} (5.8)

where $c$ is the variogram sill and $a$ is the variogram range [Deutsch and Journel, 1998]. The two experimental variograms ($\gamma_K, \gamma_f$) and the pseudo cross variogram ($\gamma_{Kf}$) were fitted to the spherical variogram model by using weighted least squares [figures 5.2-5.4]. The Cauchy-Schwarz inequality condition ensures positive definiteness:

$$|\gamma_{Kf}(h)| \leq \sqrt{\gamma_K(h)\gamma_f(h)}$$  \hspace{1cm} (5.9)

The inequality condition is enforced by using the same spherical model structure but different coefficients in all three cases [Hohn, 1998]. Constrained nonlinear optimization determines variogram model parameters by minimizing weighted sum of squared (WSS) errors [Cressie, 1985].

$$e_i = (\gamma_u - \gamma_m)^2$$  \hspace{1cm} (5.10)

$$WSS = \sum_{i=1}^{n} \left( \frac{n(h)}{\gamma_{mi}^2} \right) * e_i$$  \hspace{1cm} (5.11)

where $e_i$ is squared error, $\gamma_u$ is experimental variogram, $\gamma_m$ is model variogram, $n(h)$ is number of points at each lag, and $n$ number of lags. The inequality conditions are checked and nugget, range, and sill of $\gamma_f$ and $\gamma_{Kf}$ are adjusted to ensure a positive definite model.
Variogram Variance

Variogram estimates are uncertain because of sampling fluctuations. The variogram variance \( \text{Var}(2\hat{\gamma}(h)) \) is given as [Ortiz C. and Deutsch, 2002].

\[
\text{Var}(2\hat{\gamma}(h)) = E\left\{\left(2\hat{\gamma}(h)\right)^2\right\} - \left[E\{2\hat{\gamma}(h)\}\right]^2 \\
= E\left\{\frac{1}{n(h)} \sum_{i=1}^{n(h)} \left[z(x) - z(x + h)\right]^2\right\} - \left[E\{2\hat{\gamma}(h)\}\right]^2 \tag{5.12}
\]

where \( n(h) \) is number of data pairs separated by lag \( h \), \( z(x) \) and \( z(x + h) \) are measured data at \( x \) and \( (x + h) \). The equation estimates the point uncertainty in \( \gamma_K, \gamma_f, \) and \( \tilde{\gamma}_{Kf} \) under a multi-Gaussian assumption. Upper (95 percent) and lower (5 percent) bound variograms are estimated assuming variogram errors are lognormally distributed. To model extreme scenarios, the lower bound

![Figure 5.2: Omnidirectional experimental semivariogram and the model fit for normal score transform of hydraulic conductivity dataset.](image)
Figure 5.3: Omnidirectional experimental semivariogram and the model fit for transformed formation factor dataset.

Figure 5.4: Cross-experimental semivariogram and the model fit for normal score transform of hydraulic conductivity and transformed formation factor dataset. The variogram is set to the 5 percent at the first experimental lag and converges toward the median at higher lags [Figures 5.5-5.7; Table 5.2].
Table 5.2: Variogram model parameters

<table>
<thead>
<tr>
<th>Variable</th>
<th>Variogram</th>
<th>Model</th>
<th>Range ($\times 10^4$)</th>
<th>Sill</th>
<th>Nugget</th>
<th>Total Sill</th>
<th>Integral Range ($\times 10^4$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K$</td>
<td>Upper bound</td>
<td>Spherical</td>
<td>4.5</td>
<td>4.2</td>
<td>0.1</td>
<td>5.3</td>
<td>1.3</td>
</tr>
<tr>
<td></td>
<td>Mean</td>
<td>Spherical</td>
<td>1.5</td>
<td>0.5</td>
<td>0.5</td>
<td>1.0</td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td>Lower bound</td>
<td>Spherical</td>
<td>4.2</td>
<td>0.7</td>
<td>0.2</td>
<td>1.0</td>
<td>1.2</td>
</tr>
<tr>
<td>$f$</td>
<td>Upper bound</td>
<td>Spherical</td>
<td>4.5</td>
<td>2.6</td>
<td>0.0</td>
<td>4.6</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Mean</td>
<td>Spherical</td>
<td>1.5</td>
<td>0.4</td>
<td>0.6</td>
<td>1.0</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>Lower bound</td>
<td>Spherical</td>
<td>4.2</td>
<td>1.3</td>
<td>0.4</td>
<td>1.7</td>
<td>1.2</td>
</tr>
<tr>
<td>$K*f$</td>
<td>Upper bound</td>
<td>Spherical</td>
<td>4.5</td>
<td>3.3</td>
<td>0.4</td>
<td>4.7</td>
<td>1.2</td>
</tr>
<tr>
<td></td>
<td>Mean</td>
<td>Spherical</td>
<td>1.5</td>
<td>0.4</td>
<td>0.5</td>
<td>0.9</td>
<td>0.2</td>
</tr>
<tr>
<td></td>
<td>Lower bound</td>
<td>Spherical</td>
<td>4.2</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Univariate Kriging

Kriging uses covariance models to express data redundancy and influence. The element of covariance matrix in the $i^{th}$ row and $j^{th}$ column, $C_{ij}$, is the covariance between two points at locations $x_i$ and $x_j$, viz. $C_{ij} = C(||x_i - x_j||)$. The least squares solution to kriging weight is then $(xC^{-1}x)^{-1}(xC^{-1}y)$. The covariance matrix is estimated by using variogram or covariance models determined as discussed in the previous sections; standard methods are used to formulate the estimator and ensure unbiasedness [e.g., Goovaerts, 1997].

In this study, ordinary kriging is used to predict hydraulic conductivity in a rectangular grid of 50x 50 size covering most of Acadia parish [KT3D subroutine; Deutsch and Journel, 1998].

Simulation

The kriging error is $[z(x) - \hat{z}(x)]$ for any $x \notin$ measured data, where $z(x)$ is unknown. Simulation techniques model the error as a correlated random process. Because simulation
Figure 5.5: Estimated variogram variance of hydraulic conductivity

Figure 5.6: Estimated variogram variance of secondary data
adds back the simulated error, the variance expressed in the model (co)variograms is
preserved. Simulation is especially relevant for groundwater flow models as the high and
low values can control flow behavior [Fogg, 1986].

In this study, a sequential Gaussian simulation (sGs) reproduces the spatial
variance of hydraulic conductivity using the estimated spatial structure from the 42 data
points [SGSIM; Deutsch and Journel, 1998].

**Cokriging**

If a secondary variable is correlated with the primary variable, ordinary cokriging
can reduce estimation error. In this work, the transformed formation factor ($f$) is the
secondary variable. As in kriging, ordinary cokriging a weighted sum, but now over
observations of primary and secondary variables

$$\hat{z}(x) = \sum_{i=1}^{n_k} \lambda_{1i} K_i(x) + \sum_{j=1}^{n_f} \lambda_{2j} f_j(x)$$  \hspace{1cm} (5.13)
where \( \lambda \) is kriging weight, \( \sum_{i=1}^{n_f} \lambda_{i1} = 1 \) and \( \sum_{i=1}^{n_f} \lambda_{2j} = 0 \) for unbiased estimates. A least-squares formulation leads to a set of linear equations that can be solved for the cokriging weights [Deutsch and Journel, 1998].

**Cosimulation**

Cosimulation uses a full linear model of cross covariance. The cosimulation steps in the algorithm used in this study are: model \( \gamma_K, \gamma_f, \gamma_{Kf} \), obtain \( \gamma_f \) ensuring positive definiteness, obtain gridded transformed formation factor \( \hat{f} \) as secondary data, and calculate hydraulic conductivity estimates \( \hat{K} \) [SGSIM_FC subroutine; C.V. Deutsch, personal communication, 2003]. In the study area, the number of secondary data points is approximately the same number as of the primary data points. Thus, the information accounted of the primary data cannot be neglected when preparing the grid of secondary data. This was verified by comparing the kriged and cokriged maps of \( \hat{f} \), the secondary data. The cosimulation in this study uses a hybrid method to impose joint correlation and the correct variability:

(a) cokrige the secondary variable onto the grid,

(b) obtain a single-variable simulation of the correlated residual of the secondary variable only, using the variogram for the secondary data and equal to zero at the secondary data locations,

(c) add (b) back onto (a), then

(d) use SGSIM_FC with the normal score transform of the conductivity data and
results from (c) in place of the secondary variable simulation, and finally

(e) back-transform from normal score to hydraulic conductivity.

The aim here is to get the primary variable structure into the secondary variable via the cokriging step, with the assumption that the mean carries most of the information; the secondary residual is approximated as uncorrelated with the primary data.

**Development of the Groundwater Flow Model**

**Chicot Aquifer Models**

A regional-scale model of the Chicot Aquifer system in southwest Louisiana is being developed to examine groundwater flow dynamics in the region [Hanson et al., 2001]. High-resolution local models are being developed for subareas within the aquifer. The high-resolution MODFLOW [Harbaugh and McDonald, 1996] groundwater model of the Chicot aquifer underlying Acadia parish has five layers and 50 rows and 50 columns, resulting in a grid (block) size of approximately 0.32 sq. miles. The grid is oriented 20 degrees counterclockwise from the north-south axis to align with the flow direction [figure 3.2(b)]. A telescopic mesh refinement technique MODTMR [Leake and Claar, 1999] extracts the local model boundary conditions from the regional model results. Head boundary conditions are specified for all sides of the grid (including top and bottom). The top layer has a constant head boundary condition and the bottom layer has no flow. Initial conditions are created from the 1961 water level estimates. Pumping well types and locations was obtained from Louisiana Department of Transportation and Development's (DOTD's) Water Well GIS database [http://dotdgis2.dotd.louisiana.gov/website/lwwr_is/viewer.htm]. A total of 411 water wells (26 industrial, 27 public supply and 358 irrigation) are included in the model.
Only industrial, irrigation and public supply water wells are used in this study because these three types are responsible for more than 90 percent of the groundwater withdrawn from the Chicot aquifer [Sargent, 2002]. Yearly pumping rates were estimated by linear interpolation from the 5-year water use reports of USGS [Sargent, 2002]. The total rate was evenly distributed to the registered wells by dividing yearly pumping rate by total number of registered wells within each sector. The model was run from 1961 through 2000 and the results from the final year were used.

**Description of Aquifer Geology**

The local characterization of the Chicot Aquifer in Acadia Parish was developed using geophysical resistivity logs from 74 oil and gas exploration wells. All the geophysical logs could not be used in the cokriging method because some were outside the study area. The geology is divided into: upper confining clay; upper Chicot aquifer; dividing layer; bottom of fresh water; bottom of Chicot. Figure 3.1(b) shows a cross section of the local model along west and east direction.

**Workflow**

Modeling included these steps:

1. A grid was constructed for use with MODFLOW that simulated transient flow in a groundwater flow system.

2. Well data (K and f) were used to create images of K, using a variety of geostatistical methods.

3. The geostatistical images of conductivity were used in flow modeling, and values of specific capacity and head were generated for each model.
4. The simulated responses were analyzed statistically.

**Analysis of Variance (ANOVA)**

Four groups of simulations, each using an alternative hydraulic conductivity field created by kriging, cokriging, simulation, and cosimulation, were created with variogram at the mean and at the upper and lower bound(s). The significance of the (1) process (kriging versus simulation and cokriging versus cosimulation); (2) variables (kriging versus cokriging and simulation versus cosimulation); and (3) variogram variance (mean, 95% upper and lower bound) are tested using a multifactor ANOVA test.

The variance of the simulated models is greater than the variance from the cosimulations results. The significance of the difference was tested by comparing the variance of simulation water levels to the variance of cosimulation water levels at all three levels of variogram uncertainty using *F*-tests. Cosimulation reduces uncertainty in heterogeneity and aquifer behavior by introducing the secondary variable in the simulation process.

**Comparing Means**

Specific capacity values from different realizations of cosimulation and simulation were studied by using *t*-statistics. The *t*-test examines whether the mean specific capacity of cosimulation realizations is equal to cokriging specific capacity at the 10 percent significance level. Similarly, we tested simulation mean of specific capacity to kriging estimate.
Results and Discussion

Hydraulic Conductivity Models

Experimental (co)variograms were fitted by weighted least square estimation method for 42 hydraulic conductivity measurements and 53 transformed formation factors [figures 5.5-5.7]. The experimental variogram for hydraulic conductivity is not smooth because there are few data, a common challenge in groundwater studies. In all three cases, the total sill is equal to the transformed sample (co)variance (which is one for the transformed data). The pseudocross variogram shows correlation over a length of approximately 20,000 m, approximately one half the length of study region.

The variance of the variogram [figures 5.5-5.7] characterizes uncertainty in the variogram. Pointwise variance estimates for each lag were used to generate the extreme scenarios assuming the variogram is lognormally distributed. To get the high and low scenarios we allowed uncertainty about the sill. For all three variograms (two auto- and one crossvariogram) the lower bound variograms have longer correlation lengths and lower variability; the upper bound variograms have longer correlation as well as more variance [table 5.2]. Variogram uncertainty in the hydraulic conductivity variogram is larger than that of the secondary variable because there are more secondary data. The uncertainty in the pseudocross variogram model is much higher than the two autovariograms. The $P_5$ to $P_{95}$ ranges were used to characterize autovariogram uncertainty, whereas the pseudocross variogram was determined partly by the confidence interval and partly by the positive definiteness constraint.

The simulated and kriged hydraulic conductivity fields from coregionalized and
univariate models were created considering three levels of uncertainty in each case [figure 5.8]. As expected, the cosimulated [figure 5.8(a-c)] and cokriged [figure 5.8(d-f)] hydraulic conductivity maps have more structure than simulated and kriged maps because there is less cokriging error than kriging error; these are the basis of simulation fluctuations. The kriged estimates [figure 5.8(j-l)] are much smoother than the simulation fields [figure 5.8(g-i)]. As with the regionalized techniques, the overall structure of the cokriging and cosimulation are similar, but cosimulation has a higher variance.

Flow Model Responses

Three responses of the aquifer system are considered. The responses are (1) local averaged squared change in water level, (2) specific capacities of a selected pumping well, and (3) average water level.

Change in water level is defined as the average squared absolute water level difference obtained from the alternative models and the initial head condition \( R_i \). Averages over 20 realizations are used in stochastic cases

\[
R_i = \frac{1}{n_r} \sum_{r=1}^{n_r} \sum_{i=1}^{n_m} (h_0 - h_m)^2
\]

(5.14)

where \( h_0 \) is the initial water level, \( h_m \) is the simulated water level for the particular realization, \( n_h \) is the number of grid cells, \( n_r \) is the number of realizations. This response assesses variability in water level change. Specific capacity of well is calculated by dividing the pumping rate \( Q \) by the drawdown \( s \) in the pumping well i.e., specific capacity

\[
= \frac{Q}{s}.
\]
Figure 5.8 Distribution of hydraulic conductivity; black to white color corresponds to low (17 ft/d) to high values (2300 ft/d) in a linear scale.
A decrease in the specific capacity indicates a decline in the productivity of the well due to lower effective hydraulic conductivity field in the near-well area. A decrease in the specific capacity decreases the ability of the well to economically produce water. The specific capacity assesses influence of the hydraulic conductivity field on the ability for a well to produce water at a prescribed flow rate. The specific capacity of a well is calculated and considered as the second response ($R_2$). An average over 20 realizations is considered for simulation process.

Average water level from different flow model of alternative hydraulic conductivity fields are considered as the third response ($R_3$). Water level elevation is an indicator of aquifer depletion or aquifer potential. An average over 20 realizations is used to estimate mean and variance for stochastic cases.

The three responses are computed from the groundwater model using the alternative hydraulic conductivity fields [table 5.3]. Average water level and its fluctuation are
estimated within a 30 by 30-inner grid to avoid influences of the boundary conditions. Absolute head elevation and head difference from the kriged and cokriged conductivity models yield statistically different responses (i.e., head and specific capacity) than for the simulation models (based on t-tests; see Table 5.6).

Additional results include:

1. All responses are insensitive to variogram uncertainty for the kriged and cokriged models [Table 5.3].

2. For the (co)simulated models, increased variance in hydraulic conductivity fields (i.e., upper bound variogram) causes more fluctuation in water levels [Table 5.3]. The fluctuations are magnified as high hydraulic conductivity fields become interconnected allowing rapid movement of water to the system near the constant-head boundaries [Figure 5.9].

3. For all levels of variogram uncertainty, flow model responses indicate that coregionalized models have higher water levels than regionalized models [Table 5.3], regardless of estimation method. This implies that less sophisticated regionalized approaches are biased with respect to water level for this model and boundary conditions.

4. At the 10 percent level of significance, the variance of cosimulation responses is less than variance of simulation responses [Table 5.5]. Reduction in response variance in the coregionalized model indicates that secondary data decrease the impact of variability and thus reduce uncertainty.

5. Kriging and simulation yield similar flow responses if the correlation model is relatively smooth (i.e., the lower variogram bound). This is especially true for cokriging and cosimulation in which greater data density makes kriging error even lower.
6. *t*-tests show that the mean specific capacity of cosimulated models is significantly different than cokriged models at 10 percent level of significance [table 5.6] Similarly, mean specific capacity from the simulation realizations is significantly different from the kriged estimate.

**Table 5.3: Groundwater model flow responses using different hydraulic conductivity distributions**

<table>
<thead>
<tr>
<th>Variogram Level</th>
<th>Process</th>
<th>Variability</th>
<th>Water Level Variability (×10⁶ ft²)</th>
<th>Specific Capacity (ft²/d)</th>
<th>Average Water Level Elevation (ft)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Lower 10% CI (t-test)</td>
<td>Mean</td>
<td>Upper 10% CI (t-test)</td>
</tr>
<tr>
<td>Upper Bound</td>
<td>Simulation</td>
<td></td>
<td>6.20</td>
<td>286</td>
<td>299</td>
</tr>
<tr>
<td>Mean</td>
<td></td>
<td></td>
<td>4.88</td>
<td>287</td>
<td>293</td>
</tr>
<tr>
<td>Lower Bound</td>
<td>Coregionalized Model</td>
<td></td>
<td>4.48</td>
<td>305</td>
<td>308</td>
</tr>
<tr>
<td>Upper Bound</td>
<td>Kriging</td>
<td></td>
<td>4.25</td>
<td>309</td>
<td></td>
</tr>
<tr>
<td>Mean</td>
<td></td>
<td></td>
<td>4.21</td>
<td>310</td>
<td></td>
</tr>
<tr>
<td>Lower Bound</td>
<td></td>
<td></td>
<td>4.27</td>
<td>309</td>
<td></td>
</tr>
<tr>
<td>Upper Bound</td>
<td>Simulation</td>
<td></td>
<td>5.03</td>
<td>281</td>
<td>293</td>
</tr>
<tr>
<td>Mean</td>
<td></td>
<td></td>
<td>5.00</td>
<td>283</td>
<td>290</td>
</tr>
<tr>
<td>Lower Bound</td>
<td>Regionalized Model</td>
<td></td>
<td>4.53</td>
<td>298</td>
<td>301</td>
</tr>
<tr>
<td>Upper Bound</td>
<td>Kriging</td>
<td></td>
<td>4.41</td>
<td>305</td>
<td></td>
</tr>
<tr>
<td>Mean</td>
<td></td>
<td></td>
<td>4.43</td>
<td>304</td>
<td></td>
</tr>
<tr>
<td>Lower bound</td>
<td></td>
<td></td>
<td>4.42</td>
<td>305</td>
<td></td>
</tr>
</tbody>
</table>

Both cosimulation and simulation predict well specific capacity 5 percent lower than cokriged and kriged models, respectively. This indicates that the variance in hydraulic conductivity (as introduced by simulation) causes lower head levels, or larger drawdowns, compared with smoother (co)kriged models. Results from the cosimulated scenario show that there is a 10 percent chance that specific capacity is less than the cokriging estimate by at least 11 percent,
and specific capacity from the simulated scenario is less than the kriging estimate by at least 8 percent. However, this difference may be too small to be of practical importance.

**ANOVA Results**

The significance of the processes on the flow model response (i.e., kriging versus simulation; cokriging versus cosimulation), variable (i.e., kriging versus cokriging; simulation versus co-simulation); and variogram uncertainty (i.e., 95 percent lower limit, mean, and 95% upper limit) can be assessed using ANOVA [table 5.4]. ANOVA shows that variogram uncertainty does not have a significant effect on any flow response. On the other hand, the simulation process significantly impacts all three groundwater flow model responses (compared with kriging). Moreover, the secondary variable has a significant effect on specific capacity of well and average water level elevation (but not on average squared change).

**Table 5.4: ANOVA results on flow model responses**

<table>
<thead>
<tr>
<th>Class</th>
<th>Levels</th>
<th>Water Level Variability (ft²)</th>
<th>Specific Capacity (ft²/d)</th>
<th>Average Water Level (ft)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Pr &gt; F</td>
<td>Pr &gt; F</td>
<td>Pr &gt; F</td>
</tr>
<tr>
<td>Process</td>
<td>2</td>
<td><strong>0.03</strong></td>
<td><strong>0.01</strong></td>
<td><strong>0.04</strong></td>
</tr>
<tr>
<td>Variable</td>
<td>2</td>
<td>0.77</td>
<td>0.04</td>
<td>0.01</td>
</tr>
<tr>
<td>Variogram</td>
<td>3</td>
<td>0.27</td>
<td>0.13</td>
<td>0.19</td>
</tr>
</tbody>
</table>

Significant effects are indicated in **bold** type
Table 5.5: F-test statistic to compare simulation and cosimulation water level variances

<table>
<thead>
<tr>
<th>Variogram</th>
<th>$\sigma_s^2$</th>
<th>$\sigma_{cs}^2$</th>
<th>$F$</th>
<th>Pr &gt; $F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper Bound</td>
<td>49.5</td>
<td>36.1</td>
<td>1.33</td>
<td>0.00</td>
</tr>
<tr>
<td>Mean</td>
<td>42.9</td>
<td>37.6</td>
<td>1.14</td>
<td>0.02</td>
</tr>
<tr>
<td>Lower Bound</td>
<td>41.9</td>
<td>35.9</td>
<td>1.17</td>
<td>0.01</td>
</tr>
</tbody>
</table>

where,

$\sigma_s^2 = $ Variance of responses using simulation process

$\sigma_{cs}^2 = $ Variance of responses using cosimulation process

Table 5.6: t-test statistic to test specific capacity of simulation to kriging method

<table>
<thead>
<tr>
<th>Variable</th>
<th>$\mu_{\text{simulation}}$</th>
<th>Kriging Estimate</th>
<th>t-test</th>
<th>Pr &gt; $t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coregionalized</td>
<td>293</td>
<td>310</td>
<td>-5.9</td>
<td>0.0001</td>
</tr>
<tr>
<td>Univariate</td>
<td>290</td>
<td>304</td>
<td>-3.0</td>
<td>0.008</td>
</tr>
</tbody>
</table>

Figure 5.10: Velocity field (ft/d) from cosimulation model using (a) upper bound variogram (b) mean variogram (c) lower bound variogram.
CHAPTER 6
CAPTURE ZONE MODELING

Introduction

A capture zone is the aquifer volume that contributes water to a well within a specified time; a capture boundary is an isochrone on which travel time to the well is constant [Bakr and Butler, 2004]. Capture zone mapping can help manage groundwater resources and cleanup of contaminated aquifers.

Analytical or numerical models can be used to estimate capture zones. However, simplifying assumptions make analytical solutions inappropriate for some natural systems [e.g., Jacobson et al., 2002]. Numerical aquifer models require spatial descriptions of parameters such as hydraulic conductivity [Levy and Ludy, 2000; Cole and Silliman, 2000], porosity [Levy and Ludy, 2000], aquifer thickness [Bhatt, 1993], and recharge [Cole and Silliman, 2000]. Because aquifer properties are not known accurately, there may be large uncertainty associated with model construction and flow responses. Understanding the sensitivity of model responses to parameter uncertainty focuses modeling efforts on important parameters and increases confidence in the model.

Measurement errors and limited data cause uncertain and inaccurate descriptions of aquifer properties. Monte Carlo methods estimate uncertainty by randomly varying model properties using probability density functions [e.g., Varljen and Shafer, 1991; Franjetti and Guadagnini, 1996; Guadagnini and Franzetti, 1999; van Leeuwen et al., 1998 and 2000; Cole and Silliman, 2000]. However, many realizations may be needed to estimate response statistics if there are many, highly variable factors to be considered. Monte Carlo analysis of high-resolution models may be infeasible because these models are expensive.
In this study, a coregionalized geostatistical model and cosimulation are used to describe aquifer heterogeneity. By integrating a broad range of data, coregionalized simulation reduces the stochastic fluctuation in aquifer properties; reducing the fluctuations decreases the number of realizations required to assess uncertainty [Rahman et al., in review].

Typically, Monte Carlo groundwater studies do not consider uncertainty in the geostatistical model itself. However, Feyen et al. [2001] considered variogram parameter uncertainty in capture zone modeling using unconditional hydraulic conductivity fields. In contrast, the approach proposed in this paper uses estimates variogram uncertainty analytically [Ortiz C. and Deutsch, 2002] and uses conditional methods.

Prior information on plausible correlation and variance helps in two ways: it regularizes the problem by adding data, and it specifies meaningful distributions to use in sampling procedures. Feyen et al. [2002, 2003.a, 2003.b] used a Bayesian approach to analyze capture zones, incorporating priors for the mean and covariance of transmissivity. A Bayesian approach allows the use of prior information to update the posterior probabilities in light of data [Hilborn and Mangel, 1997]. However, they used noninformative priors. Here, the priors for variogram parameters (i.e., range, sill and nugget) are modeled informatively with beta distributions.

Feyen et al. [2001] used generalized likelihood uncertainty estimation to analyze stochastic well capture zones, weighting transmissivity using head observations. That method requires many realizations. Here, the spatial structure of the variables is analyzed using likelihood to compare simulated and experimental variograms. A Bayesian approach
improves the description of variogram uncertainty by combining prior information with likelihood.

Although many studies consider capture zones, few use field datasets and model multiple properties. Bhatt [1993] examined sensitivity of capture zone to aquifer properties (e.g., transmissivity, hydraulic gradient, porosity, and thickness) using an analytical model with no field data. Van Leeuwen [1998, 2000] studied capture zone sensitivity varying transmissivity only. This paper examines three properties -- hydraulic conductivity, porosity, and aquifer thickness -- to assess the impact that their variability has on capture zone size and shape.

Although recharge is commonly a significant factor affecting aquifer behavior [Cole and Silliman, 2000], it is not examined in this study because a clay layer overlies the aquifer and no major water bodies interact with this portion of the aquifer [Hartono and Willson, 2005].

In this study, aquifer properties are generated using geostatistical methods that are consistent with available data. The groundwater simulations use cosimulated hydraulic conductivity fields, simulated porosity fields, and kriged thickness models. Uncertainty in the properties is addressed by creating models over the range of the uncertainties in the geostatistical models for the aquifer properties. The approach can model coregionalized fields.

This paper presents a dataset from the Chicot aquifer, and discusses statistical and flow analyses. Data Used in This Study describes basics of measurement and interpretation for this area of the Chicot aquifer. Then, Geostatistical Method analyzes variogram uncertainty using a Bayesian approach, and geostatistical simulation methods for aquifer
properties are described. In *Groundwater Modeling*, coregionalized aquifer property models are used in a steady-state capture zone model. Important findings are amplified in Results and Discussion.

**Data Used in This Study**

The Chicot aquifer underlies much of southwest Louisiana including Acadia parish. Available data within the Acadia parish study area (25 km²) include hydraulic conductivity and resistivity logs [figure 3.1 and 3.2]. The resistivity logs [figure 3.1(b)] are used to derive transformed formation factor, porosity, and aquifer thickness.

Hydraulic conductivity values are calculated from pumping tests using a semi-empirical method [Carlson et al., 2003; Rahman et al., 2005]. Forty-two values are available in the Acadia Parish study area [figures 3.2].

Because few pump test data are available, secondary data are used to improve the hydraulic conductivity estimates. Fifty-three formation factor \((F)\) values are calculated from resistivity logs in the same 25-km² area [figures 3.1 and 3.2]. These data are still sparse, and are not collocated with pumping data; these features complicate analysis and geostatistical modeling.

The resistivity data, (i.e., formation factor, \(F\)) are used to derive a transformed variable \(K_F\) which will be used to cosimulate the hydraulic conductivity. Formation factor and hydraulic conductivity are related using the Kozeny-Carman equation [Carman, 1956]. The values for pore geometry, \(a\), and cementation coefficient, \(m\), in the Archie equation are estimated by maximizing the short-distance covariance between hydraulic conductivity \((K)\) and transformed formation factor \((K_F)\) using nonlinear regression. This
gives a version of the Kozeny-Carman equation in terms of the formation factor and Archie equation parameters,

\[ K_F = \frac{\rho g}{\mu} \left( \frac{F^{m_k} a^{m_k}}{\left( F^{m_k} - a^{m_k} \right)^2} \right) d_m^2 \frac{180}{1} \]  

(6.1)

where porosity is assumed to follow the Archie equation [Archie, 1942],

\[ \phi = \left( \frac{a}{F} \right)^{\frac{1}{m}} \]  

(6.2)

For this dataset, \( \hat{a}_K = 1.76 \) and \( \hat{m}_K = 1.64 \). The short-lag crosscovariance for this model is an approximate upper bound for the crossvariogram nugget. For this portion of the Chicot aquifer, the average particle diameter is \( d_m = 0.43 \) mm (1.22 in phi units; USGS unpublished data files). Additional details are discussed in chapter 5. The subscripts on the Archie parameters [equation 6.1] indicate that the regression was to maximize correlation with hydraulic conductivity. The formation factors are also used to estimate porosity using the Archie equation. For the porosity calculations, the coefficients are indicated as \( a_\phi \) and \( m_\phi \). These are not the same as for the transformed formation factor; \( a_K \) and \( m_K \) are intended to maximize the linear correlation between the transformed formation factors (\( K_F \)) and the hydraulic conductivity. Thus, \( a_K \) and \( m_K \) are confounded with factors such as particle size and do not solely reflect porosity. Porosity is calculated using \( a_\phi \) and \( m_\phi \) from the Humble formula for unconsolidated sand [Asquith and Gibson, 1982]. Because the use of the correlations for transformed formation factor and porosity are different, different Archie parameters \( a \) and \( m \) are used.
Geophysical logs are also used to estimate the aquifer thickness. There are 54 observations [figures 3.1 and 3.2] of aquifer thickness in the same study area.

**Geostatistical Methods**

This section presents variogram computation and simulation, likelihood estimates of simulated variograms, and Bayesian posterior probability for the simulated variograms.

**Variogram Models**

A variogram model is specified using a vector of parameters, \( \theta \), which includes ranges, rotation, sill, and nugget. The mean semivariogram is \( \gamma(h, \bar{\theta}) \) where \( h \) is the separation vector or lag and \( \bar{\theta} \) is the vector of variogram parameter means. The experimental semivariograms are calculated from [Matheron, 1971]

\[
\gamma_Z(h) = \frac{1}{2} E \left[ (Z(u + h) - Z(u))^2 \right] 
\]

(6.3)

where \( Z(u + h) \) and \( Z(h) \) are measured values at coordinate \( (u + h) \) and \( u \) respectively, and \( h \) is the lag separation distance. The variogram parameters are then estimated by regression yielding \( \hat{\theta} \) which is used as the estimator of \( \bar{\theta} \).

For all cases considered here, the spherical variogram models are fit to the data [figure 6.1(a-c)]. The spherical variogram model is where \( c \) is the variogram sill and \( r \) is the variogram range [Deutsch and Journel, 1998]. For this isotropic model, \( \theta_1 = r, \theta_2 = c \).

\[
\gamma(h, \hat{\theta}) = \begin{cases} 
\frac{3|h|}{2r} - \frac{1}{2} \left( \frac{|h|}{r} \right)^3, & |h| \leq r \\
0, & |h| > r
\end{cases} 
\]

(6.4a)

\[
\gamma(h, \hat{\theta}) = c, \quad h \geq r 
\]

(6.4b)
None of the hydraulic conductivity data are collocated with the formation resistivity data (i.e., the transformed formation factor, $K_F$). Thus, instead of using the crossvariogram, the coregionalized model for the hydraulic conductivity field uses a pseudocrossvariogram [Clark et al., 1989]

$$\hat{\gamma}_{12}(h) = \frac{1}{2} E \left[ \left( Z_1(u + h) - Z_2(u) \right)^2 \right]$$  \hspace{1cm} (6.5)

where $Z_2$ is the secondary variable (here, transformed formation factor, $K_F$). Pseudocrossvariogram models must satisfy Schwartz’s inequality for all lags [Hohn, 1998]

$$\left| \gamma_{21}(h, \hat{\theta}) \right| \leq \sqrt{\gamma_{11}(h, \hat{\theta}) \times \gamma_{22}(h, \hat{\theta})}$$  \hspace{1cm} (6.6)

where 1 corresponds to the primary variable and 2 corresponds to the secondary variable.

The pseudocrossvariogram is also fit with a spherical model [figure 6.2(a-b)]. The range of the secondary property variogram and pseudocrossvariogram are the same as range of hydraulic conductivity to ensure positive definiteness. The variance of a variogram, $\text{Var}(2\gamma(h, \hat{\theta}))$, scales the error for each lag estimate. This can be calculated using [Ortiz C. and Deutsch, 2002]

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{variograms.png}
\caption{Variograms for primary aquifer properties with lower and upper bound.}
\end{figure}
Figure 6.2: Variograms for secondary property, transformed formation factor, and pseudocross variogram with lower and upper bounds.

\[ Var(2\gamma(h, \hat{\theta})) = E\left(\left(2\gamma(h, \hat{\theta})\right)^2\right) - \left[E\left(2\gamma(h, \hat{\theta})\right)\right]^2 \]

\[ = E\left(\frac{1}{n(h)} \sum_{i=1}^{n(h)} [Z(u) - Z(u + h)]^2\right)^2 - \left[E\left(2\gamma(h, \hat{\theta})\right)\right]^2 \] (6.7)

where \( n(h) \) is the number of data pairs separated by lag distance \( h \); \( Z(u) \) and \( Z(u + h) \) are measured data at \( u \) and \( (u + h) \) coordinates respectively. The pointwise variogram variances allow generating the lower and upper bound scenarios assuming variogram sill is log normally distributed. For all three variables, including secondary and pseudocross variogram, the lower bound variograms have longer correlation lengths with lower variability and the upper bound variograms have longer correlation with more variance [figure 6.1(a-c), 6.2(a-b)]. Uncertainty in the porosity variogram is much less than the other variograms. The uncertainty in the secondary variable and pseudocross variogram are largest because the confidence interval is determined jointly by the positive definite constraint and estimated variogram variance.
**Variogram Model Priors**

Simulated variograms for hydraulic conductivity, porosity, and aquifer thickness and secondary and pseudocross variograms define (co)regionalized models for aquifer properties. The variogram simulation uses prior distributions of variogram model parameters.

Variogram models are fit to experimental variograms to obtain the median parameter vector $\overline{\theta}$ and the lower (5 percent) and upper (95 percent) bounds (the bounds are estimated from variogram variance assuming that the variogram at each lag is log-normally distributed). Pointwise variogram variance estimates for each lag are used to generate the extreme scenarios assuming the variogram sill is log normally distributed. These statistics stipulate the priors for the variogram parameter vector, i.e., range, sill, and nugget [Rahman et al., 2005]. The estimates of lower, median, and upper for each variogram parameter are used to fit beta cumulative density functions [Abramowitz and Stegun, 1972]

$$F(x) = \frac{\int_{0}^{x} x^{\alpha-1} (1-x)^{\beta-1} \, dx}{\int_{0}^{1} x^{\alpha-1} (1-x)^{\beta-1} \, dx} \quad (6.8)$$

where $x$ is a random variable ranging from 0 to 1; $\alpha$ and $\beta$ are greater than zero. The beta distribution has a finite domain and can be modified to reproduce a wide range of means, variances, and skewness. In this study, the beta distributions are fit to the median, lower and upper bounds by minimizing the sum of squared error between the point estimates and the fitted model. Although these distributions are rather crude approximations, they comprise only the priors and will be updated (Posterior Density of Variogram, below). Variogram uncertainty models imply priors for variogram parameters [figure 6.3(a-i) and figure 6.4(a-d)]. In all cases parameter values are transformed to $[0,1]$ to fit the beta distributions.
**Variogram Ranges**

The variogram range of hydraulic conductivity varies between 4,500 and 14,000 m.; hydraulic conductivity ranges between 13,000 and 14,000 m have low probability. Porosity ranges vary between 4,500 and 10,000 m (8,000 to 10,000 have very low probability) and thickness range varies from 6,000 to 13,000 m.

**Variogram Sills**

The variogram sill of hydraulic conductivity ranges from 0.5 to 4.2 (ft/d)$^2$ (0.7 to 4.2 have low probability), the porosity sill varies from 0.3 to 0.8 (0.7 to 0.8 have very lower probability), and the thickness sill is between 0.4 and 4.0 ft$^2$ with (0.5 to 4.0 have very low probability).

**Variogram Nuggets**

The hydraulic conductivity nugget varies from 0.2 to 1.1, porosity nugget is between 0.2 and 0.7, and thickness nugget varies between 0.2 and 0.6. In all cases the nuggets were distributed smoothly and did not exhibit the long tails of other variogram parameters.

**Variogram Simulation**

One thousand variogram models $\gamma(h, \theta)$ are simulated using a factorial combination of these variogram parameters [figure 6.5(a-c)]. The coregionalized model uses the same correlation range as the primary variograms and is constrained by the positive definiteness requirement. This constraint implies that only sill and nugget can be varied for the secondary and pseudocrossvariograms [figure 6.6(a-b)].

The simulated porosity variogram has a narrower range than other aquifer properties; the thickness variogram has a wider range [table 6.1].
Figure 6.3: Prior distributions of variogram parameters (normalized range, sill, and nugget) for hydraulic conductivity, porosity and aquifer thickness. The lines show fitted Beta distribution and points show prior estimates.

The pseudocrossvariogram has yet more variation as few data points are available to estimate crosscovariance between primary and secondary properties. This simulation assumes that the variogram parameters are independent. However, appropriate parameter correlations will be introduced through likelihood calculations.
Figure 6.4: Prior distribution of variogram parameters (normalized sill and nugget) for secondary and pseudocross variogram. The lines show fitted Beta distribution and points show our prior estimates.

**Variogram Likelihood**

Likelihood is the probability of an observation given a model. For example, in the case of variograms, the likelihood of a vector of variogram parameters, $\theta$, is

$$
\lambda(\theta) = \frac{p(\gamma | \theta)}{\int p(\gamma | \theta) d\Omega}
$$

(6.9a)

where $\Omega$ is the space of the parameter vector $\theta$ and the $Z$ subscript is used for each variable. Likelihood enables calculation of confidence bounds on the distribution by estimating the mean and variance of variogram parameters and comparing each possible model to the experimental variogram [Hilborn and Mangel, 1997].
Figure 6.5: Simulated variogram for hydraulic conductivity, porosity and aquifer thickness. A random subsample of $10^2$ variogram is shown out of $10^3$ for clarity. All distances are in meters.

Figure 6.6: Simulated variogram for secondary and pseudocross variogram. All distances are in meters.

The mean and variance estimates are subject to error. Assuming that this error is normally distributed, and neglecting the normalizing term in the denominator of equation (6.9a),

$$
\hat{\lambda}(\theta) \propto \prod_{i=1}^{n} \frac{1}{\sigma_{Z}(h_i, \theta)} \exp \left[ -\frac{[\gamma_{Z}(h_i, \theta) - \gamma_{Z}(h_i, \overline{\theta})]^2}{\sigma_{Z}^2(h_i, \theta)} \right] \quad (6.9b)
$$

where

$\hat{\lambda}(\theta)$ likelihood of each variogram model or parameter set,

$\gamma(h, \theta)$ simulated variogram model,
\( \gamma(\mathbf{h}, \overline{\theta}) \) mean state from eqn. (3),

\( \sigma(\mathbf{h}, \overline{\theta}) \) prior standard deviation of the variogram parameters

Table 6.1: Variogram uncertainty models estimated from variogram mean and variance.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Variogram</th>
<th>Model</th>
<th>Range (km)</th>
<th>Sill</th>
<th>Nugget</th>
<th>Total Sill</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K )</td>
<td>Lower bound</td>
<td>Spherical</td>
<td>13</td>
<td>0.7</td>
<td>0.2</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Median</td>
<td>Spherical</td>
<td>5</td>
<td>0.5</td>
<td>0.5</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Upper bound</td>
<td>Spherical</td>
<td>14</td>
<td>4.2</td>
<td>1.1</td>
<td>5.3</td>
</tr>
<tr>
<td>( K_f )</td>
<td>Lower bound</td>
<td>Spherical</td>
<td>13</td>
<td>1.3</td>
<td>0.4</td>
<td>1.7</td>
</tr>
<tr>
<td></td>
<td>Median</td>
<td>Spherical</td>
<td>5</td>
<td>0.4</td>
<td>0.6</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Upper bound</td>
<td>Spherical</td>
<td>14</td>
<td>2.6</td>
<td>2.0</td>
<td>4.6</td>
</tr>
<tr>
<td>( K*K_f )</td>
<td>Lower bound</td>
<td>Spherical</td>
<td>13</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Median</td>
<td>Spherical</td>
<td>5</td>
<td>0.4</td>
<td>0.5</td>
<td>0.9</td>
</tr>
<tr>
<td></td>
<td>Upper bound</td>
<td>Spherical</td>
<td>14</td>
<td>3.3</td>
<td>1.4</td>
<td>4.7</td>
</tr>
<tr>
<td>( \phi )</td>
<td>Lower bound</td>
<td>Spherical</td>
<td>8</td>
<td>0.7</td>
<td>0.2</td>
<td>0.9</td>
</tr>
<tr>
<td></td>
<td>Median</td>
<td>Spherical</td>
<td>5</td>
<td>0.4</td>
<td>0.6</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Upper bound</td>
<td>Spherical</td>
<td>11</td>
<td>0.8</td>
<td>0.7</td>
<td>1.0</td>
</tr>
<tr>
<td>( T )</td>
<td>Lower bound</td>
<td>Spherical</td>
<td>6</td>
<td>0.5</td>
<td>0.2</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>Median</td>
<td>Spherical</td>
<td>7</td>
<td>0.6</td>
<td>0.4</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Upper bound</td>
<td>Spherical</td>
<td>13</td>
<td>4.0</td>
<td>0.5</td>
<td>4.5</td>
</tr>
</tbody>
</table>

where
\( K \) is hydraulic conductivity
\( K_f \) is transformed formation factor
\( K*K_f \) is for Pseudocross variogram
\( \phi \) is porosity
\( T \) is aquifer thickness

The subscript \( i \) denotes a summation over lags, not a component of \( \mathbf{h} \). Each simulated variogram, \( \gamma(\mathbf{h}, \theta) \) is compared to the experimental variogram, \( \gamma(\mathbf{h}, \overline{\theta}) \) assuming that deviations in variogram parameters are normally distributed \([\text{mean}, \gamma(\mathbf{h}, \overline{\theta}); \text{standard deviation}, \sigma(\mathbf{h}, \overline{\theta})]\).
The likelihood for the entire variogram is estimated as the product of the individual likelihoods for each lag, assuming that lags are independent. While not rigorous, but this assumption is acceptable and makes analysis possible [Ortiz-C. and Deutsch, 2002].

**Posterior Density of Variogram**

Variogram parameter uncertainty can be reduced by incorporating prior knowledge. Bayesian methods allow updating this prior in light of additional data [Denison et al., 2002]. The posterior density combines the a priori distribution for the variogram, $P_{\text{prior}}(\theta)$, with the probability of observing data given the variogram, $P(\theta | \theta)$,

$$P_{\text{posterior}}(\theta | \theta) \propto P(\theta | \theta) \times P_{\text{prior}}(\theta)$$  \hspace{1cm} (6.10)

or

$$P_{\text{posterior}}(\theta | \theta) = \frac{P(\theta | \theta) \times P_{\text{prior}}(\theta)}{P(\theta)}$$ \hspace{1cm} (6.11a)

Here, the posterior probability is assumed to be defined by the 1000 simulated variograms. Therefore,

$$P_{\text{posterior}}(\theta) = \frac{\sum_{i=1}^{1000} P(\theta | \theta) \times P_{\text{prior}}(\theta)}{\sum_{i=1}^{1000} P(\theta)}$$ \hspace{1cm} (6.11b)

The choice of prior stipulates information about the unknown variogram. Prior probability for range, sill, and nugget are estimated from their corresponding fitted beta distribution [equation 6.8]. Because the variogram model parameters are assumed independent, the prior for the variogram model is

$$P_{\text{prior}}(\theta) = P_{\text{prior}}(R) \times P_{\text{prior}}(S) \times P_{\text{prior}}(N)$$ \hspace{1cm} (6.12)
where $\mathbf{R}$, $\mathbf{S}$, and $\mathbf{N}$ are the vector of range, sill and nugget of simulated variogram model. The required subroutines are part of public domain statistical software [R Development Core Team, 2004; Ribeiro and Diggle, 2001].

Likelihood profiles for each of the variogram parameters illustrate model plausibility in light of available data [Hilborn and Mangel, 1997]. Likelihood profiles are estimated for all variogram parameters. Likelihood surface plots for sill vs. nugget combination are contoured by calculating likelihood over the grid of values while keeping range as fixed. The likelihood profile of hydraulic conductivity suggests that the most likely range is near or equal to 4,000 m [figure 6.7(a)]. The most probable variogram sill [figure 6.7(b)] for conductivity is 0.5. Similarly, the most likely nugget for the variogram is 0.5 or higher [figure 6.7(c)]. The likelihood profile for the range of porosity is rather flat, but it shows [figure 6.7(d)] that range is likely higher that 6,000 m. The sill of porosity [figure 6.7(e)] has probable values less than or equal to 0.45, and the corresponding nugget [figure 6.7(f)] is likely to be greater than 0.7. High nugget for porosity reflects large small-scale variation that is expected in porosity. The range of thickness is less than 15,000 m [figure 6.7(g)], and its sill is likely less than 1 [figure 6.7(h)]. Likely values for thickness nugget are less than 0.35 [figure 6.7(i)], reflecting higher short-range correlation.

For the secondary variogram most likely values of sill and nugget [figure 6.8(a-b)] are near 0.5 and 0.8 respectively. For pseudocrossvariogram most likely sill is 2 and nugget [figure 6.8(c-d)] is 0.8 or greater; this high nugget reflect the softness of the correlation between the primary and secondary variable. Likelihood surfaces show the plausibility of sill and nugget combination in light of data, and whether there is any correlation between the sill and nugget. The likelihood surface for hydraulic conductivity [figure 6.9(a)] shows little
correlation between sill and nugget; the most likely sill is less than 1 and nugget is between 0.4 and 0.7.

Figure 6.7: Log-likelihood profile of variogram parameters for hydraulic conductivity, porosity and aquifer thickness. All ranges are in meters; for hydraulic conductivity and thickness sills and nuggets are in (m/d)^2 and m^2. For porosity sills and nuggets are dimensionless.
The porosity variogram [figure 6.9(b)] has sill and nugget negatively correlated. The thickness variogram likelihood surface [figure 6.9(c)] suggests no correlation between sill and nugget. Lower sills are more likely, but likelihood does not depend strongly on the nugget over the prior value of [0.35, 0.55]. The secondary variogram likelihood surface shows [figure 6.10(a)] negative correlation and lower sills and nuggets combination are more likely. The low variance implies that the secondary variable, the transformed formation factor, is more uniform than hydraulic conductivity as more data are available.
The pseudocrossvariogram likelihood [figure 6.10(b)] shows no correlation between sill and nugget and higher sill-nugget combinations are more likely. The pseudocrossvariogram parameter variance is high because there are few data at short lags.

Comparison between prior and posterior densities shows [table 6.2] that the prior expectations of variogram data have been systematically altered by the experimental variogram calculations. The mean and standard deviation of integral range are less after the update. The reduction in geostatistical parameter variance implies decreased of among variogram parameters.

The integral range is the area under the correlogram curve

\[
R_i = \int_0^\infty \rho(h)dh
\]  

(6.13)

where \( \rho \) is the correlogram and \( h \) is the separation distance.

Alternatively,

\[
R_i = \int_0^R \left(1 - \frac{\gamma(h)}{S}\right)dh
\]  

(6.14)

where \( \gamma(h, \theta) \) is the semivariogram and \( S \) is the sill. The integral range of each variogram is tabulated with the corresponding posterior distribution [table 6.2].

Integral range quantifies statistical fluctuations and correlation of a stochastic model [Lantuejoul, 2002]. Here, integral range is used to select variograms with three different levels of correlation; sorting on this single parameter indirectly preserves the expected continuity in thickness compared to other aquifer properties.
Figure 6.9: Log-likelihood surface plot of variogram parameters for hydraulic conductivity, porosity and aquifer thickness. For hydraulic conductivity and thickness sills and nuggets are in (m/d)² and m² respectively. For porosity sill and nugget are dimensionless.
Figure 6.10: Log-likelihood surface plot of variogram parameters for secondary and pseudocross variogram. Sills and nuggets of the two variograms are in (m/d)^2.

For each variable, a set of three variograms corresponding to 5, 50, and 95 percent is extracted from the posterior cumulative density of integral range [figures 6.11(a-c) and 6.12(a-c)]. The quantiles of integral range give different variograms. Among the variograms of similar integral range, the one with highest likelihood (range, figure 6.7(a, d, g); sill and nugget, figure 6.9(a, b, c)] is chosen as the model to represent that level of integral range. The same integral range may correspond to distinct $\theta$. Therefore, samples of all variograms with integral ranges in a particular interval are grouped and compared to samples for other intervals of the integral range using ANOVA.

Analysis of variance [ANOVA; Fisher, 1935] separates important “treatment” or systematic effects from random errors, unmodeled factors, and each other. A “treatment” is a set of conditions created for the experiment that correspond to the probability level of an aquifer property of this study [Montgomery, 1997].
Figure 6.11: Posterior distribution of integral range for hydraulic conductivity, porosity and aquifer thickness. The dashed lines indicate 5%, 50% and 95% interval. For hydraulic conductivity and thickness integral ranges are in (m/d)^2 and m^2 respectively. For porosity integral ranges are dimensionless.

An $F$-test compares the variation within and groups. Here, a large $F$ would indicate that the integral range carries little information about variogram parameter variability, and vice versa. ANOVA is also used in response analysis in this study.

Similar integral ranges for different variograms are grouped to examine variance of variograms within and among groups. Integral range is shown to be a meaningful grouping
criterion for the effects of spatial correlation on flow responses (Use of Experimental Design section). A correlation matrix for integral range, variogram range, sill, and nugget shows [Table 6.3] that integral range is highly correlated with range and moderately correlated with sill and nugget. Integral range is reproducing much of the total covariance of the variogram parameters, but not all of it. Collapsing a 3-dimensional problem (range, sill, and nugget) to one-dimensional (integral range) is a simplification that may not be reasonable in many cases. Here, it significantly eases the combinatorics of many different models for different aquifer properties.

**Simulation and Estimation of Aquifer Properties**

**Hydraulic Conductivity**

Forty-two hydraulic conductivity and 53 transformed formation factor values are linearly related in this dataset. Coregionalized simulation integrates the formation factor transform to improve hydraulic conductivity models. Geostatistical simulation is used for conductivity because, unlike kriging, it reproduces variance as well as correlation range. This is desirable because variance and correlation range jointly affect the flow behavior [e.g., Gelhar and Axness, 1983]. The cosimulation process uses auto- and crosscovariances [Rahman et al., in review].

Hydraulic conductivity simulations use lower (5 percent, $K_1$), median (50 percent, $K_2$) and upper bound (95 percent, $K_3$) of auto- and pseudocrossvariograms from the posterior densities of integral range. Twenty realizations of the hydraulic conductivity fields sample stochastic fluctuation for each set of variogram models.
A coregionalized simulation procedure [SGSIM_FC.FOR subroutine: C.V. Deutsch, personal communication, 2003] was modified to write a binary file of realizations of hydraulic conductivity for stochastic MODFLOW [Ruskauff, 1994].

**Porosity**

The porosity field is constructed from sand resistivity values obtained from 53 geophysical logs in the area using the Humble formula for unconsolidated sand [Asquith, 1980]. Porosity fields are simulated at the lower (5 percent) ($P_1$), median (50 percent) ($P_2$) and upper (95 percent) ($P_3$) bounds of uncertainty using sequential Gaussian simulation and models from the posterior distribution of integral range.

**Thickness**

The aquifer thickness is estimated by kriging. Kriging is suitable for thickness because thickness varies smoothly whereas conductivity does not. The geophysical logs provide estimates of thickness at 64 locations. Models are kriged at lower (5 percent) ($T_1$), median (50 percent) ($T_2$) and upper bound (95 percent) ($T_3$) of the posterior of integral range.

**Groundwater Modeling for the Chicot Aquifer**

**Flow Model**

The Chicot aquifer in southwestern Louisiana is a major source of fresh water. The Chicot comprises upper and lower sands [figure 3.1(a)]. The upper Chicot is interbedded sand and gravel 40 m to 98 m thick within the study area. The lower Chicot varies between 98 m and 240 m thick. A 15 m thick impermeable layer separates the upper and lower sands, acting as a barrier to flow. The upper Chicot is more permeable than the lower [Rao et al.,
A thick clay layer overlies and confines the upper Chicot. The groundwater system is bounded below by low permeability sediments [Hanson et al., 2001].

A MODFLOW [Harbaugh and McDonald, 1996] regional model of the Chicot Aquifer system has been constructed for the region [Hanson et al., 2001]. That model has been updated by increasing grid resolution, and incorporating more detailed geology and aquifer stresses [Hartono and Willson, 2005].

A more detailed, local MODFLOW grid underlying Acadia parish is extracted from the regional model using telescopic mesh refinement [figure 3.2], which extracts local boundary conditions from the regional model using linear interpolation [e.g., Ward et al., 1987]. The local model has 50 rows and 50 columns (1000 m by 1000 m) with variable thickness. Leakance of the aquifer is zero, allowing no recharge across the overlying clay layer.

The model includes 411 water wells (26 industrial, 27 public supply and 358 irrigation). A GIS-based technique calculates pumping rates for irrigation, industrial, and public supply sectors using various spatial (e.g., land cover, crop type) and temporal data (e.g., rainfall, land use, crop growth stage) to estimate irrigation groundwater demand [Hartono and Willson, 2005]. Public supply and industrial usage are from USGS records. Locations and depths of water wells are from the Department of Transportation and Development GIS water well database. Here, year 2000 rates are used in a steady state model.

Capture Zone Model

Particle tracking delineates capture areas in complex aquifer systems [e.g., Varljen et al., 1991; Leuween et al., 1998; Levy and Ludy, 2000]. MODPATH [MODPATH, Pollock
et al., 1989] uses a three-dimensional grid of horizontal rectangular cells and assumes a confining layer with one-dimensional, steady state flow. Cell-by-cell flow rates from MODFLOW are used to compute the particle paths through the model domain.

A high-capacity well is chosen for capture analysis [figure 6.13] because it is near the center of the study area and is isolated from other wells, minimizing the influences of boundary conditions. The capture area of the well is computed using one particle per cell.

Figure 6.13: Two scenarios (model run 5 and 23) of capture zone boundary, at 90% confidence limit, of the study well.

Forward particle tracking is used; reverse particle tracking is not available in this software. The simulation covers 20 years at steady state. The probability distribution of the capture zone is estimated from 20 realizations of hydraulic conductivity field and MODFLOW-MODPATH results.
Table 6.2: Prior versus posterior density of integral range

<table>
<thead>
<tr>
<th>Integral Range</th>
<th>$K$</th>
<th>$\phi$</th>
<th>$T$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\mu$</td>
<td>$\sigma$</td>
<td>$\mu$</td>
</tr>
<tr>
<td>Prior</td>
<td>4000</td>
<td>3316</td>
<td>650</td>
</tr>
<tr>
<td>Posterior</td>
<td>3500</td>
<td>1276</td>
<td>600</td>
</tr>
</tbody>
</table>

Table 6.3: Correlation of integral range with variogram parameters for hydraulic conductivity.

<table>
<thead>
<tr>
<th>$R_i$</th>
<th>Range</th>
<th>Sill</th>
<th>Nugget</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_i$</td>
<td>1.0</td>
<td>0.9</td>
<td>0.4</td>
</tr>
<tr>
<td>Range</td>
<td>0.9</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Sill</td>
<td>0.4</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Nugget</td>
<td>-0.2</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

**Model Response as Capture Zone Compactness**

Each model set uses a different combination of $K$, $P$ and $T$ corresponding to 3 levels (high, median, and low integral range for each aquifer property); this yields $3^3$ or 27 model sets. Twenty realizations of hydraulic conductivity per model set address stochastic fluctuations.

Capture zone compactness is used to measure capture zone shape as the area ($A$) for a given perimeter ($P$). This can be written in dimensionless form as

$$C_d = \frac{4\pi A}{P^2}$$

(6.15)
Thus, a compactness of 1 gives perfectly circular capture zone indicating the most compact shape and a small value (i.e., approaching zero) indicates a long thin shape capture zone, or the least compact shape.

**Workflow**

The following steps are followed to estimate capture zone sensitivities:

1. Estimate variogram mean and variance, and assign probability distributions (here, beta distributions) to the variogram parameters (range, sill, and nugget).

2. Draw random samples from the distributions of each parameter and use combinations of all parameters to simulate variograms.

3. Calculate prior, likelihood and posterior probability for simulated variograms from step 2.

4. Calculate integral ranges for the simulated variograms from step 2 and tabulate in $P_{\text{posterior}}(\theta)$.

5. Draw 5, 50, and 95 percent variogram from posterior probability of integral range.

6. Create geostatistical realizations for each of the $3^3$ factor combinations.

7. Simulate capture zones using MODFLOW and MODPATH and compile results

8. Perform ANOVA

**Results and Discussion**

**Use of Experimental Design**

In experimental design, a series of tests or model runs are performed by systematically changing the input variables (or factors) of the system, observing the
response, and inferring the principal causes for changes in the output response [Montgomery, 1997]. In this study, groundwater simulations with alternative geostatistical parameters are run and the capture zone characteristics are calculated. Each of the aquifer properties (hydraulic conductivity, porosity and thickness) is simulated at three levels (5, 50, and 95 percent) of integral range.

The use of integral range to categorize models is investigated using ANOVA. Three groups are defined [Table 6.4], centered on cumulative probabilities of 5, 50, and 95 percent for the hydraulic conductivity spatial model. In each group, some numbers of variogram models within a small error \( (p - \varepsilon \leq p \leq p + \varepsilon) \) bound at the centerpoint are selected. Hydraulic conductivity is chosen for the test as it is the most sensitive property. These variogram models within the error limit (0.01) at each level of integral range comprise the groups. The error width is chosen as reasonable numbers of variogram models are found within the group for ANOVA test. Cosimulated hydraulic conductivity fields are constructed for \( N = (N_{0.05} + N_{0.5} + N_{0.95}) \times N_R \) cases where \( N_R \) is the number of realization. 20 realizations are used in this case. Flow models are constructed for \( (N_{0.05} + N_{0.5} + N_{0.95}) \) cases and capture zone compactness was tabulated for analysis. If within-group variance of capture zone compactness is small compared to between-group variance, then integral range is an acceptable method for defining model categories. \( F \)-tests show [Table 6.5] that variances of model responses within the groups are statistically insignificant \( (p = 0.23) \) and variances among groups are statistically significant \( (p = 0.01) \). The test implies that any variogram from a group of similar integral range is equally representative, and selecting models from various integral ranges reproduces most of the response variance.
Table 6.4: Groups of integral range for ANOVA test

<table>
<thead>
<tr>
<th>Groups</th>
<th>$K_{0.05}$</th>
<th>$K_{0.5}$</th>
<th>$K_{0.95}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>10</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>$\mu$</td>
<td>1725</td>
<td>3900</td>
<td>9410</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>5</td>
<td>11</td>
<td>374</td>
</tr>
</tbody>
</table>

where

- $N$ is the number of variogram within a group
- $\mu$ is the mean of integral range
- $\sigma$ is the standard deviation of integral range

Table 6.5: Probability effect is random from $F$-tests on what with groups defined by posterior probability of integral range.

<table>
<thead>
<tr>
<th>Class</th>
<th>$K_{Pr&gt;F}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variance of responses within</td>
<td>0.22</td>
</tr>
<tr>
<td>groups</td>
<td></td>
</tr>
<tr>
<td>Variance of responses</td>
<td>0.01</td>
</tr>
<tr>
<td>among groups</td>
<td></td>
</tr>
</tbody>
</table>

where, significant effects are indicated in **bold** type.

**Response Analysis**

Capture zone area [Figure 6.13] and compactness from each experiments of the 27 used as responses [Table 6.6]. The sensitivity of aquifer properties (i.e., hydraulic conductivity, porosity, and thickness) to capture zone model is assessed using analysis of variance, taking capture zone area and compactness as model responses. At the 10 percent significance level, hydraulic conductivity and aquifer thickness models have significant impact on capture area [table 6.7]. Hydraulic conductivity models have significant impact on capture zone uncertainty as measured by compactness [table 6.7]. Though aquifer thickness models are not significant for capture area compactness ($p=0.06$, table 6.7) at the 10 percent
significance level, this variable is nonetheless retained in the analysis. These models analyze numerical experiments that are free of random, unlike “true” experiments.

**Effects of Stochastic Fluctuations**

Model responses such as capture area over perimeter, \( \frac{4\pi A}{P^2} \), for different number of hydraulic conductivity realizations are calculated and plotted against square root of number of realizations, \( \sqrt{N_{\text{realizations}}} \). In this analysis, porosity and thickness realizations are not varied. Model responses for 20 realizations are taken as the finest case, \( \varepsilon_R = \left| \frac{4\pi A}{P^2} - \frac{4\pi A_{\text{finest}}}{P_{\text{finest}}^2} \right| \). Increasing the number of hydraulic conductivity realizations from 8 to 20 (finest case) only accounts for 6 percent of response uncertainty. On the other hand, changing hydraulic conductivity model from the low continuity bound (level 1) to the high bound (level 3) explains 31 percent of capture zone uncertainty.

Uncertainty incorporated by different geostatistical models is much larger than uncertainty incorporated by realizations. That is, uncertainty studies that examine only fluctuations of a fixed correlation model may greatly underestimate response uncertainty. Moreover, it has been shown that other, deterministic effects such as shale drapes and concretions may overwhelm stochastic fluctuations in hydraulic conductivity [e.g., White et al., 2004].

**Effects of Porosity Variability**

The importance of using multiple realizations for porosity model is investigated using \( t \)-tests. Capture zone compactness from 6 realizations of porosity models at lower and upper levels of all integral ranges are compared. The effect of response fluctuations between realizations of the porosity field in modeling experiment is not significant by \( t \)-tests (10 percent level). Therefore, only hydraulic conductivity requires multiple realizations.
Table 6.6: Mean capture zone model responses from factorial design experiment.

<table>
<thead>
<tr>
<th>Model Run</th>
<th>Hydraulic conductivity</th>
<th>Porosity</th>
<th>Thickness</th>
<th>Capture area</th>
<th>Capture length</th>
<th>Circularity ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>38</td>
<td>25</td>
<td>0.77</td>
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<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>63</td>
<td>37</td>
<td>0.59</td>
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<tr>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>57</td>
<td>33</td>
<td>0.64</td>
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<tr>
<td>4</td>
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<td>2</td>
<td>1</td>
<td>41</td>
<td>26</td>
<td>0.75</td>
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<tr>
<td>5</td>
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<td>2</td>
<td>28</td>
<td>20</td>
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<tr>
<td>6</td>
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<td>8</td>
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<td>11</td>
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<td>104</td>
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<td>3</td>
<td>91</td>
<td>50</td>
<td>0.47</td>
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<tr>
<td>13</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>72</td>
<td>41</td>
<td>0.54</td>
</tr>
<tr>
<td>14</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>40</td>
<td>25</td>
<td>0.79</td>
</tr>
<tr>
<td>15</td>
<td>2</td>
<td>2</td>
<td>3</td>
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<tr>
<td>16</td>
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<td>3</td>
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<td>1</td>
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<td>89</td>
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<td>3</td>
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<td>59</td>
<td>0.41</td>
</tr>
<tr>
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<td>3</td>
<td>3</td>
<td>3</td>
<td>91</td>
<td>46</td>
<td>0.55</td>
</tr>
</tbody>
</table>
Table 6.7: ANOVA results on 20 years of capture zone model responses i.e., capture area $(A)$ and compactness $\left(\frac{4\pi \times A}{P^2}\right)$.

<table>
<thead>
<tr>
<th>Class</th>
<th>Levels</th>
<th>$A$ Pr &gt; F</th>
<th>Compactness Pr &gt; F</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K$</td>
<td>3</td>
<td>0.004</td>
<td>0.001</td>
</tr>
<tr>
<td>$\phi$</td>
<td>3</td>
<td>0.102</td>
<td>0.141</td>
</tr>
<tr>
<td>$T$</td>
<td>3</td>
<td>0.005</td>
<td>0.06</td>
</tr>
</tbody>
</table>

where, significant effects are indicated in **bold** type.
CHAPTER 7
CONCLUSIONS AND RECOMMENDATIONS

The hydraulic conductivity distribution affects ground water flow model predictions. Because field data are typically sparse compared to model resolution, geostatistical techniques are used to translate field measurements to densely gridded data. Geophysical data such as formation factor can be used to improve predictions of coregionalized hydraulic conductivity distribution. Noncollocated, secondary data are used in the coregionalized model with a pseudocross variogram. Results and interpretations are based on changes in the groundwater model responses as simulation process, variables, and variogram level are altered; the significance of these effects are examined using ANOVA. The use of a coregionalized field (e.g., cosimulated or cokriged) significantly changes the flow model response compared to the univariate models. For all responses, the results from the (co)simulated fields are significantly different than those from the (co)kriging methods. Heterogeneity in simulated hydraulic conductivity fields creates well-connected regions of contrasting conductivity, leading to locally higher water velocities. Therefore, cosimulation should be used instead of cokriging to capture velocity variability in models; this is especially relevant for capture analysis and contaminant transport. Use of cosimulated hydraulic conductivity distribution in the flow model may be more significant in more heterogeneous systems. Improved estimates of hydraulic conductivity with reproduction of heterogeneity and uncertainty estimates could affect ground water resource management for heavily pumped local systems. Variogram uncertainty on groundwater model flow response is relatively insignificant for the correlation structure, variance level, and data configuration examined.
A geostatistical method for analyzing data uncertainty was applied in order to estimate sensitivity of parameters that affect capture zone behavior. The method utilized in this study to incorporate variogram uncertainty is more effective for capture zone modeling compared to traditional Monte Carlo method where a large number of realizations, requiring storage and time costs, would be involved. Several aquifer properties fields were generated using the available data and confidence bounds associated with the uncertainty estimates. Predictions were improved by incorporating prior knowledge through a Bayesian approach. The predicted fields are used in a groundwater model to solve for head and velocity fields. In this study, prior knowledge and geological knowledge were integrated into the approach. The sensitivity method allows changing spatial structure of parameters in a sequential manner while keeping it consistent with available data and its variance. The method is also applied to a coregionalized field. ANOVA results show that the capture area in this system is most sensitive to the hydraulic conductivity and aquifer thickness models and least sensitive to the porosity model. The ANOVA results also show that capture area compactness in this system is most sensitive to the hydraulic conductivity and porosity models and least sensitive to the aquifer thickness model. Realizations based on a fixed variogram model assess only a small portion of uncertainty. Examining alternative geostatistical models does account for uncertainty. The sensitivity analysis presented in this study is reliable as it allows for comparison of multiple aquifer properties, the stochastic fluctuation due to property uncertainty, calibration to flow and geophysical data, and geostatistical parameter certainty. The approach developed here to account for uncertain aquifer properties is especially convenient for a complex aquifer system. Finally, the method to assess variogram uncertainty
can also be used to model predictive stochastic capture zones at a minimum of storage and time.

Data integration is challenging because different levels of support between primary and secondary data need to be correlated in various ways. In this dissertation, we have developed methodologies to integrate non-collocated sparse geophysical data and investigate uncertainty to better understand aquifer heterogeneity. Future study can extend this research by integrating groundwater head observations with hydraulic conductivity measurements and electrical resistivity data as the secondary soft data. A Bayesian geostatistical approach can be adopted to fuse the primary and secondary data to better interpret the hydraulic conductivity distribution statistically. Cokriging can be used to obtain the conditional mean and covariance of hydraulic conductivity by using spatial correlation and cross-correlation among the inferred and measured hydraulic conductivity data. The probability of the cokriged hydraulic conductivity distribution can be used as the prior information in the Bayesian method. A likelihood function can be obtained via the assumption that errors between the observed and calculated heads have a multi-Gaussian distribution. Therefore, the posterior probability can result as the integration of three data types in a statistical form. Through Bayesian geostatistics, the error propagation and conditional uncertainty from the original data to the estimated results can be investigated.
REFERENCES


Archie, G. E. (1942): The Electrical Resistivity Logs as an aid in Determining some Reservoir Characteristics, Transactions of AIME.


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## APPENDIX: DATA

Table 1: Hydraulic Conductivity Data

<table>
<thead>
<tr>
<th>Easting</th>
<th>Northing</th>
<th>Hydraulic Conductivity(ft/d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>550753.1</td>
<td>3339827.7</td>
<td>2297</td>
</tr>
<tr>
<td>565988.0</td>
<td>3330800.9</td>
<td>260</td>
</tr>
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<td>566475.8</td>
<td>3327483.3</td>
<td>945</td>
</tr>
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</tr>
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<td>3319743.7</td>
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</tr>
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VITA

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