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A SOLUTION TO AN INVERSE PROBLEM OF GROUNDWATER FLOW USING STOCHASTIC FINITE ELEMENT METHOD

by

MAS AGUS MARDYANTO

A thesis
presented to the
Faculty of Graduate and Postdoctoral Studies
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In the name of Allah, Most Gracious, Most Merciful.

To my late parents,

"My Lord, be merciful to them just as they brought me up with kindness and affection."
(Qur'an; 17:24)

and

To my beloved wife, Titin, and son, Amarendra.

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All praise is to Allah. "O my Lord, grant me the power and ability that I may be grateful for your favor which You have bestowed upon me and my parents, and that I may do righteous good deeds, such as please You, and make my offspring good." (Qura'n; 46:15)

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ABSTRACT

A sustainable groundwater management is imperative because suitable groundwater resources are progressively diminishing. The groundwater management in an area requires reliable forecasting. For forecasting, it is necessary to have site-specific information on the hydrological characteristics of geological formation including the groundwater flow parameters such as hydraulic conductivity. The parameters of groundwater flow can be obtained by laboratory testing or field measurements. The resulting parameters obtained by those measurements, however, are only representative of the local characteristics of an aquifer corresponding to the sampling points. Considering the heterogeneous characteristic of geologic formations, it would be most desirable to obtain the distribution of parameters in an aquifer for the purpose of reliable forecasting. This objective can be achieved by, first, taking hydraulic head measurements at various observation wells as well as the hydraulic conductivity measurements at specified locations and then analyzing all field measurements using a stochastic inverse groundwater flow model.

For modeling, computer programs are required. Many computer programs developed for this purpose are available in the market. However, most of the programs for solving groundwater flow problems deal with deterministic processes. Computer programs for the analysis of stochastic processes are commercially available; however, most of these programs consider only the steady state flow. Therefore, a computer program for solving stochastic, transient groundwater flow problems in heterogeneous porous media is needed.

In this study, a stochastic finite element method is used to solve an inverse problem in groundwater flow. The adjoint states method combined with cokriging method is used to

estimate the distribution of hydraulic conductivities in an area where hydraulic heads and hydraulic conductivities are measured at some locations. This method starts with obtaining the expected hydraulic heads in the entire study domain at different times. Then, the adjoint states at different times are calculated. Using both calculated values as input, the Jacobians that are needed for the development of covariance matrices of hydraulic heads at different times and the cross-covariance matrices between hydraulic heads at different times and hydraulic conductivities in the aquifer are calculated. Using the maximum likelihood estimate method (MLE), which utilizes all covariance and cross-covariance matrices obtained from the previous step, the statistical parameters (mean, variance, and correlation scale) of the model are estimated. Using the statistical parameter values and all observed values of hydraulic heads at different times and all measured hydraulic conductivities, the distribution of hydraulic conductivity in the entire study domain is estimated.

An attempt is made in this thesis to verify the computer program by utilizing two hypothetical problems as verification cases. In some parts of the aquifer, mostly at locations around the observation wells, the resulting hydraulic conductivity distributions have the same pattern with the "true" distribution patterns in both cases of verification. The values of L2-norms calculated by using the "true" and estimated values of log hydraulic conductivity are 0.18 and 0.57 for Case 1 and 2, respectively.

Regression analyses are also conducted to determine the strength of correlation between the "true" and estimated values of hydraulic conductivity at all nodes and between the observed and estimated values of hydraulic conductivity at observation wells in Case 1 and Case 2 of verification. The correlations between the "true" and estimated values of hydraulic conductivity at all nodes are weak in both cases of verification. However, the observed and estimated values of hydraulic conductivity at observation wells are strongly correlated.

Predictions are made using MODFLOW. Steady state and transient flow problems are analyzed. In the steady state and transient flow problems, the results of the forward analyses using the "true" and estimated values of hydraulic conductivity do not differ significantly for both cases of verification.

Data from two field problems are analyzed as an application of the computer program. The estimated values of hydraulic conductivity are found to be within the range of the observed values given in the original reports. These applications can be considered as a part of the validation of the method.

Considering the results of both case studies, it appears that the computer program developed in this study can be used with reasonable success to estimate the hydraulic conductivity distribution in real aquifers. As will be explained in the discussion of the results, however, the effect of zonation needs to be investigated further.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

GLOSSARY

b : the thickness of an aquifer

d_{ij} : the distance between point x_i and x_j

F : the expected value of Y, E[Y]

f : the variation of Y about the mean value.

$G(x,t)$: a user-chosen function

g_0 : given functions defined on sections of flow region (Ω)

g_1, g_2 : given functions defined on parts of boundary (Γ_1, Γ_2)

H : the expected head, $E[\phi]$

h : the variation of hydraulic heads about the mean value

JB :The Jacobian matrix

p : the number of observation time

LG : the log likelihood function

l_Y : the log hydraulic conductivity correlation scale

n : unit vector in the direction normal to Γ_2

Q : the discharge or recharge

R : the flow region

S : the storage coefficient

t : time

t_0 : the initial time

t_p : an observation time

x,y : spatial variables

x_l : the location of an observation well

Y : logarithm of the hydraulic conductivity, log K

z : the measurement vector of Y and/or ϕ

Ω : a performance function

$\zeta(x,y)$: a basis function

$\xi_{l,k}$, λ_m: co-kriging coefficients

$\delta(\,)$: the dirac delta function

θ : the statistical parameter vector

ν : the Lagrange multiplier

μ_Y : the expected value of Y, E[Y]

σ_Y^2 : the log hydraulic conductivity variance

ϕ : the total hydraulic head

ψ : the adjoint state

Cov_{YY} : the covariance of log hydraulic conductivity

Q_D : the measurement covariance matrix

$Q_{D,\phi\phi}(t_k, t_k)$: the covariance matrix of observation head of time t_k

$Q_{D,\phi\phi}(t_{k1}, t_{k2})$: the covariance matrix between heads at observation times t_{k1} and t_{k2}

$Q_{D,\phi Y}(t_k)$: the head-log K measurement cross-covariance matrix

LIST OF THE GREEK SYMBOLS / GREEK ALPHABETS

Capital Symbol	Lower Case Symbol	Name	Capital Symbol	Lower Case Symbol	Name
Α	α	Alpha	Ν	ν	Nu
Β	β	Beta	Ξ	ξ	Xi
Γ	γ	Gamma	Ο	ο	Omicron
Δ	δ	Delta	Π	π ϖ	Pi
Ε	ε	Epsilon	Ρ	ρ	Rho
Ζ	ζ	Zeta	Σ	σ ς	Sigma
Η	η	Eta	Τ	τ	Tau
Θ	θ ϑ	Theta	ϒ	υ	Upsilon
Ι	ι	Iota	Φ	ϕ φ	Phi
Κ	κ	Kappa	Χ	χ	Chi
Λ	λ	Lambda	Ψ	ψ	Psi
Μ	μ	Mu	Ω	ω	Omega

CHAPTER 1

INTRODUCTION

1.1 Problem Statement

Groundwater is an indispensable source of fresh water for industrial, agricultural, domestic, and other purposes of consumption. The quantity as well as the quality of groundwater is important. A shortage of groundwater will be experienced if withdrawal of water is more than natural recharge in an aquifer. In addition, seawater intrusion and land subsidence are possible side effects of groundwater depletion. Therefore, a sustainable groundwater management is imperative.

The groundwater management in an area requires reliable forecasting. For forecasting, it is necessary to have site-specific information on the hydrological characteristics of geological formation. The information required for an analysis includes the geometric dimensions, boundary conditions, amount of discharge from wells, natural extraction (evapotranspiration), replenishment (infiltration), and the parameters such as hydraulic conductivity, storativity or specific yield. The boundary conditions are specified as hydraulic head or flux across the boundaries of the study domain.

The parameters of groundwater flow can be obtained by laboratory testing or field measurements. The laboratory testing can be done on samples brought from the field. Procedures for laboratory test for soils and rocks are described in the Annual Book of ASTM Standards (ASTM, 1993). In the field, pumping tests can be used to obtain those parameters (Dawson and Istok, 1991). However, the resulting parameters obtained by those measurements are only representative of the local characteristic of an aquifer corresponding to the sampling point for laboratory testing or to a small area around the point of field measurement.

For the determination of the flow characteristics of the whole aquifer, many measurements have to be taken. Richard (2002) emphasized that if the number of measurement points of parameters of an aquifer is not sufficiently large, the meaningful estimates of parameters cannot be obtained. The number of measurements, however, becomes extremely large if one wants to be sure of measuring all possible variability in parameters and boundary conditions. The cost of aquifer characterization will increase with increasing number of measurements. In addition, the aquifer might be damaged if the number of measurements becomes excessive.

In general, groundwater flows through geologic formations with heterogeneous characteristics. Flow properties, such as the hydraulic conductivity, vary over space due to the variation of aquifer properties. The variation in aquifer properties is mainly caused by the variation in the physical environment of deposition. In heterogeneous formations, a significant amount of variation in the value of hydraulic conductivity can occur within a distance of 10^{-2} metres to 10^{3} metres. An example of the variability of measured hydraulic conductivity in the field can be seen in Figure 1.1 (Gelhar, 1993). In addition, the groundwater table fluctuates with time. The precipitation, infiltration, evapotranspiration, recharge to and discharge from an aquifer also vary in space and time. An example of the variability of infiltration rate is shown in Fig. 1.2 (Gelhar, 1993). It is clear from these examples that the soil properties in the field may vary rapidly within a small distance. Consequently, it is difficult or almost impossible to treat these kinds of variability by a deterministic approach because there is no exact value to be used as input for a parameter.

Stochastic methods are occasionally employed to deal with the uncertainties in groundwater flow problems (Gelhar, 1993; Abdin, 1996; Dagan, 2002). Kaluarachchi et al. (1990) and Myers (2002) stated that stochastic methods give better and more meaningful results compared to the deterministic methods in many surface and groundwater flow studies. This approach provides probabilistic predictions regarding the behaviour of aquifers by considering that the parameters are random variables (de Marsily, 1986; Gelhar, 1986; Dagan, 2002). The probability density functions (pdf) of parameters in an area are provided as input. The resulting equations are in the form of differential equations of dependent variables. Therefore, the dependent variables obtained from these equations can also be represented as probability density functions (Dagan, 2002). In spite of its advantages, the stochastic modeling is not used frequently as a tool for groundwater management problems including the parameter identification problems. It is important to use this technique as a tool to model real field problems and to demonstrate its usefulness in the analysis of practical engineering problems.

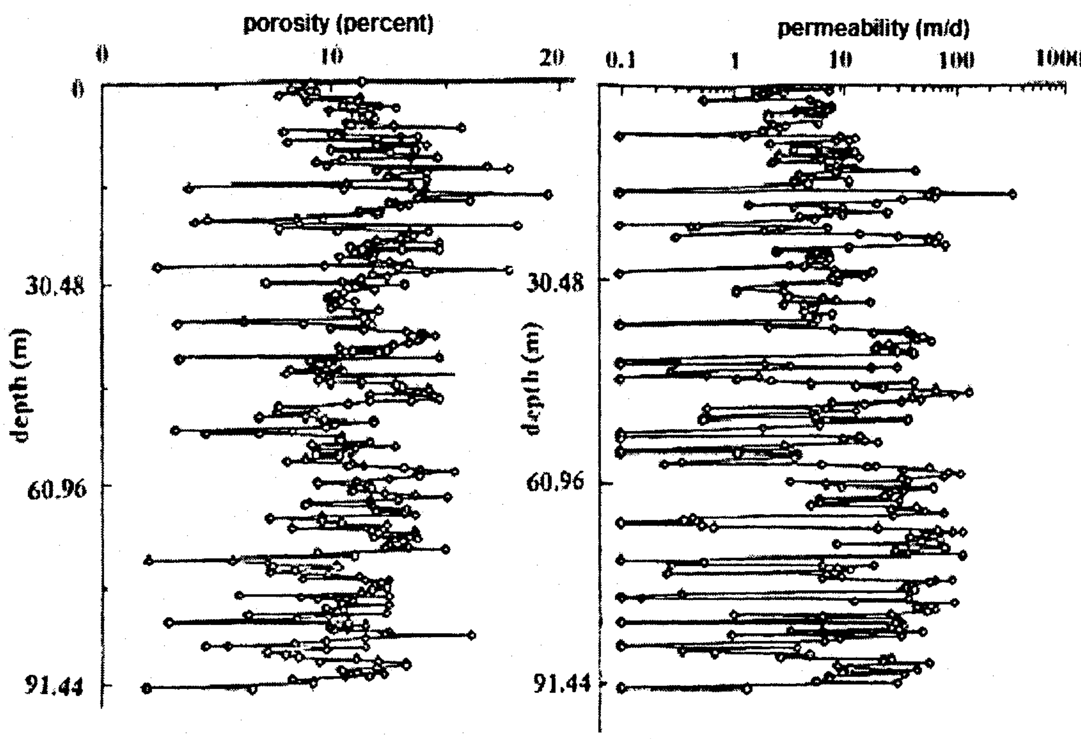


Figure 1.1 Permeability and porosity (for a sandstone aquifer) of cores collected at 1-ft intervals from boreholes (ILO56) in the Mt. Simon aquifer in Illinois (Gelhar, 1993, where the data is taken from Bakr, 1976)

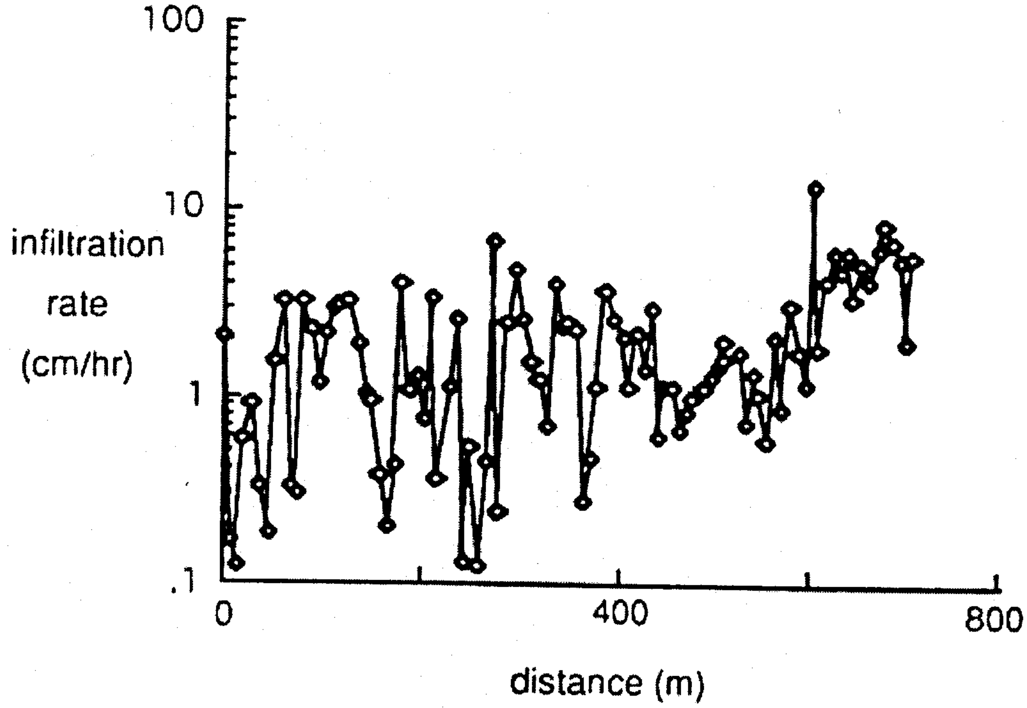


Figure 1.2 Infiltration rate observed at 25-ft intervals at the ground surface in a recent alluvial deposit at Rio Grande near Socorro, New Mexico (Gelhar, 1993; where the data is taken from Gelhar et al., 1983)

Various researchers developed stochastic models, which include Monte Carlo simulation, Random Walk approach, Transfer function methods, Lagrangian perturbation techniques, Eularian perturbation analysis, Spectral perturbation methods, Eularian-Lagrangian theory, and Markov Chain model. Some of these models are briefly explained in the subsequent chapter.

A groundwater flow problem can be solved analytically only for simple boundary conditions and for a porous media with homogeneous physical properties. For an aquifer with complex boundary conditions and physical properties, it is difficult or may be impossible to employ an analytical method. Therefore, it becomes necessary to develop numerical models.

Many researchers used the finite element method to solve groundwater flow problems (Kaluarachchi and Parker, 1989; Sudicky, 1989; Li et al., 1999). Some other researchers included stochastic processes in their analyses (Sagar, 1978; Graham and McLaughlin, 1989a, 1989b, 1991; Li, 1998; Li and Graham, 1998; Salandin and Fiorotto, 1998). Most researchers worked with forward problems and only a few dealt with inverse problems especially related to the stochastic processes. The forward methods require, as input, the physical parameters and boundary conditions. The results of the forward analysis, however, would not be reliable if the input data were not representative of field conditions. Therefore, forward methods of analysis require calibration of input data to produce predictions comparable to the actual behaviour of an aquifer. Usually, the calibration is done by trial and error.

Inverse methods in groundwater modeling are utilized to obtain representative values of the physical parameters and/or boundary conditions of an aquifer. For example, the input data required, in addition to the initial and boundary conditions, for the inverse analysis of hydraulic conductivities can be hydraulic heads at the observation wells as well as the amount of discharge and/or recharge. Automatic fitting replaces the trial and error approach to find the physical parameters of the aquifer. The results of the inverse solution can be used for reliable forecasting (Sun, 1999). According to de Marsily (1986), the inverse analysis is the most important phase of constructing groundwater flow models.

For numerical modeling purposes, a computer program needs to be developed. There are only a few commercially available programs, which can be used to solve inverse problems in groundwater studies (MODFLOWP, PEST, GEOPACK, SOILPARA, UCODE, and GROUNDWATER VISTAS). These commercial programs are described in Chapter 2. However, most of these programs deal with the inverse problems in deterministic sense except the last program in the list. The stochastic nature of the groundwater flow is considered only in GROUNDWATER VISTAS, which uses the Monte Carlo simulation method. Nonetheless, the stochastic analysis using this program is possible only for steady state flow problems.

1.2 Research Objective

The main objective of this study is to develop a stochastic finite element program for the analysis of groundwater flow. The program will be used to solve an inverse problem where the probabilistic values of the hydraulic conductivities corresponding to different regions of an aquifer will be determined from the hydraulic head and hydraulic conductivity measurements taken at a limited number of points. This research will be restricted to two-dimensional, confined aquifer flow systems. Only the fully saturated flow will be considered. Moreover, the program will be used in the analysis of real field problems for the validation purposes.

1.3 Scope of Study

The inverse solution method will be used to estimate the parameters of the groundwater flow by utilizing the hydraulic heads and hydraulic conductivities measured at selected points. Both the hydraulic heads and hydraulic conductivities will be treated as random variables. To estimate the parameters, the adjoint state equation will be utilized as described by Sun and Yeh (1992). The resulting equations will be solved using the Galerkin Finite Element algorithm.

To achieve the objectives of this study, a set of FORTRAN and MATLAB programs will be developed. These computer programs are listed below.

1. A program to calculate expected hydraulic heads, adjoint states, and Jacobians
2. A program to estimate statistical parameters
3. A program to estimate hydraulic conductivities in the study domain

The details of these computer programs are given later in this thesis.

CHAPTER 2

LITERATURE REVIEW

2.1 Models for Groundwater Flow

In groundwater flow studies, it is usually difficult or maybe impossible to determine the response of an aquifer to future activities by doing laboratory and field experiments. In stead, groundwater flow models, that are representation of real groundwater flow systems or processes (Bear, 1979; Konikow and Bredehoef, 1992; Kitanidis, 1997), can be developed to predict the behaviour of groundwater flow in an aquifer.

The groundwater flow models can be categorized as physical models (porous media models, miscellaneous analog models, electrical analog models), and mathematical models (Todd, 1980). In physical models, a small-scale model is assumed to represent the actual field conditions or process. In a mathematical model, the actual field conditions are expressed with mathematical equations. In the mathematical modeling, a computer program is usually needed to solve the flow problem, especially when dealing with complex and large domains. Both physical and mathematical models can possibly simulate the groundwater flow in a given domain; however, the actual conditions in the field and flow processes are usually simplified in both models (Bear, 1979).

Mathematical models have some advantages. (1) They can handle complex conditions of aquifer systems. The complexity of aquifer systems comes from the heterogeneity and anisotropy conditions of hydraulic conductivities, the irregularity of geometric shapes of aquifers, different types of boundary conditions, and the variability of discharge/recharge to and from aquifers. (2) They are easy to calibrate; i.e. one can adjust the values of some parameters so that the response of the modeled aquifer (water table or hydraulic head) becomes similar to the real response. Therefore, engineers generally use mathematical models in most basin studies (Sun, 1999). However, since most parameters of groundwater flow are measured indirectly and boundary conditions cannot be defined precisely, it is not easy to make a good prediction of the groundwater flow behavior using mathematical models (Kitanidis, 1997).

2.2 Uncertainties in the Solution of Groundwater Flow Problems

The main reasons for the uncertainties in the solution of the groundwater flow problems are listed below.

- The hydraulic properties of subsurface soils such as the hydraulic conductivity, coefficient of storage, and porosity are highly variable in most cases (Gelhar, 1993).
- The amount of recharge of groundwater from rainfall is not known accurately.
- The recharge or discharge of groundwater from and to a stream is not known definitely since the water levels in both the subsurface and the stream also vary.
- Temperatures, which influence the value of hydraulic conductivity, vary in time and space.

There are three possibilities in dealing with the natural variability in an aquifer (Gelhar, 1993). These are

(1) Collect field data at each point when the physical conditions change and use these data in a numerical model that includes the effect of all possible causes of variability. This approach is impractical because it results in extensive damage to the aquifer.

(2) Ignore the variability in parameters and treat the aquifer system as homogeneous everywhere. This approach means, "Do nothing" about the variability.

(3) Treat the variability of the hydraulic properties as random variables. This third approach is called "stochastic" and this approach is summarized in Fig. 2.1 (Gelhar, 1993). This figure shows that a solution to a stochastic problem can be obtained through three possible paths. They are

(a) Treat parameters of the hydraulic properties as being random and include this randomness into the classical groundwater flow equation. The work in this thesis is under this category.

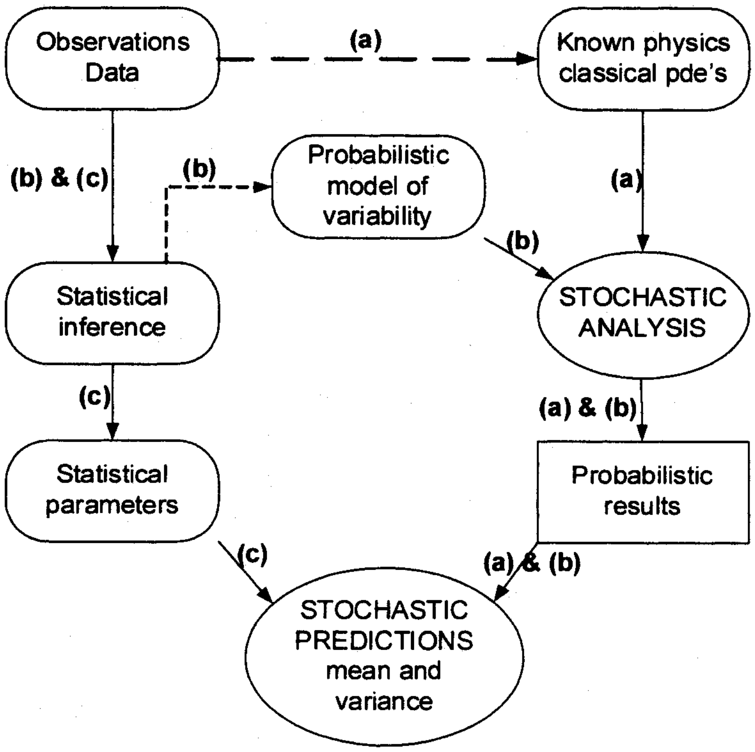


Figure 2.1 Summary of the stochastic approach (from Gelhar, 1993)

(b) Identify a suitable probabilistic model of observation and data through the process of statistical inference, then, estimate the model parameters by stochastic analysis. The work of Adamowski and Hamory (1982) is under this category. They developed a stochastic input-output model of groundwater level fluctuation in a region and its impact to the river flow using a spectral time series analysis. They found that a second-order autoregressive moving average, ARMA (2, 0), model was adequate to describe the input-output process of a groundwater scheme.

(c) Process the observations and data and predict the outcome through probabilistic analysis without considering the groundwater flow equation. This approach is commonly used in determining the extreme flow such as flood and draught in surface water hydrology based on historical data of rainfall obtained from many weather stations (see Gelhar, 1993). In groundwater flow studies, this approach can also be used to predict the fluctuation of groundwater table due to accretion, discharge, and evapotranspiration based on historical data of groundwater management in a region.

2.3 Stochastic Models

The term stochastic process refers to a process that contains a set of random variables (Shahin et al., 1993). This process needs to have not only its probability distribution function but also a joint probability distribution between all points in space to characterize the process completely. The outcomes of stochastic processes cannot be predicted with certainty. They can only be expressed by probabilistic measures. An example of a stochastic process is the variability of hydraulic head in an aquifer. It varies in time and/or space due to the variation of recharge or discharge. The variability of the hydraulic head cannot be predicted exactly; however, it can be defined by its temporal mean and variance. If the hydraulic heads in space are correlated, their spatial covariance can also be defined.

Various researchers have conducted studies in stochastic modeling. The list provided by Li (1998) with some additional, more recent references, are given below.

1. Monte Carlo simulations (Warren and Price, 1961; Freeze, 1975; Smith and Freeze, 1979a, 1979b; Ammozegar-Fard et al., 1982; Espinoza, 1997; Salandin and Fiorotto, 1998; Wong, 1998; Wood and Kavvas, 1999).
2. Random Walk approaches (Ahlstrom et al., 1977;Tompson et al., 1989; Valocchi et al., 1989).
3. Transfer function methods (Jury et al., 1982, 1986).
4. Lagrangian perturbation techniques (Dagan, 1982b, 1984, 1986, 1987; Rubin and Dagan, 1987a, 1987b; Rubin and Bellin, 1994; Neuman and Zhang, 1990; Zhang and Neuman, 1990).
5. Eularian perturbation analysis (Gelhar, 1976; Bakr et al. 1978; Gutjahr et al., 1978; Gelhar et al., 1979; Mizell et al., 1982; Gelhar and Axness, 1983; Yeh et al.,

1985a, 1985b; Mantoglou and Gelhar, 1987a, 1987b, 1987c; Graham and McLaughlin, 1989a, 1989b, 1991; Graham and Tankersley, 1994; Kapoor and Gelhar, 1994a, 1994b; Li and Graham, 1998).

6. Spectral perturbation methods (Gelhar, 1986; Robin, 1991; Abdin, 1996).
7. Eularian-Lagrangian theory (Neuman, 1993; Zhang and Neuman, 1995a, 1995b, 1995c, 1995d).
8. Markov Chain model (Elfeki, 1998).

The general steps of Monte Carlo Simulation and Perturbation methods will be given below because of their relevance to the present research.

Monte Carlo Simulation Method

Monte Carlo Simulation is a well-known method dealing with stochastic processes. The Monte Carlo simulation method has been used in the study of groundwater flow by many authors such as Wong, 1998; and Wood and Kavvas, 1999. In this method, a large number of realizations that follows a certain distribution function have to be generated. Unlike the perturbation and spectral methods, in the Monte Carlo method the probability distribution function of random variables in a domain has to be known prior to the analysis (de Marsily, 1986). The generated realizations, that are fully determined and known, are then used as input in the numerical analysis to solve the governing equation. The resulting ensemble of dependent variables is then analyzed statistically for each point, i.e., the mean, variance, histogram, and distribution function (de Marsily, 1986; Kitanidis, 1997). The Monte Carlo method may be considered as the most powerful method since it can simulate almost all natural phenomena including groundwater flow. Moreover, this method provides results that are comparable to the closed form solutions. For this reason, the Monte Carlo simulation method is often used as a tool for validation of other stochastic methods (Abdin, 1996). However, since it needs to take into consideration a very large number of realizations (50 to several hundreds or thousands, de Marsily, 1986) it consumes a lot of time. Additional details can be found in de Marsily (1986) and Kitanidis (1997).

As mentioned before, in using this method one needs to generate realization of spatial random field variables such as hydraulic conductivity distribution in a domain. The most common method to use in generating these random field variables in groundwater studies is the turning bands method (Matheron, 1973; Mantoglou and Wilson, 1982; Tompson et al., 1989). In this method, a one-dimensional process with a zero mean and a covariance function along multiple lines is determined. The covariance function along multiple lines is a reduced version of a two- or three-dimensional covariance function. By making use of this covariance function, a one-dimensional second-order stationary discrete process is generated along each line. Then, all discrete values generated on the lines are projected orthogonally onto points on the field where one wants to generate the values of random variables. The assigned values on the field are the weighted average of the projected values from all available lines. An example of the two- dimensional case, taken from Mantoglou and Wilson (1982), is presented in Figure 2.2. Let W be a point in a two-dimensional field P in which one wants to generate a value of the random variable. An arbitrary origin O in space R^n is chosen. Many lines are drawn outward starting from the origin O as shown in the figure. On each line a unit vector is indicated. For instance, in Figure 2.2, θ_i is an angle between the reference line χ and a line i. θ_i is uniformly distributed between 0 and 2π. Then, one needs to generate a second-order stationary one-dimensional discrete process along line i. This discrete process has a zero mean and a covariance function $C_1(\zeta)$ in which ζ the coordinate on line i. The vector, x_W, representing the position of point W in the field P is projected orthogonally onto line i. ζ_{Wi} is the projection of the vector x_W and its value is equal to an inner product $x_W.u_i$ where u_i is the unit vector on line i. The value of the one dimensional-discrete process on the line i, $z_i(\zeta_{Wi})$, is assigned to point W. The same procedure is repeated for all the lines in the field. The covariance function $C_1(\zeta)$ is used to generate an independent one dimensional realization for each line. The number of assigned values $z_i(\zeta_{Wi})$ at point W is equal to J where J is the number of lines and i = 1, 2, …, J. Then, the assigned values at point W can be calculated using the following equation.

$$z_s(\underline{x}_W) = \frac{1}{\sqrt{J}} \sum_{i=1}^{J} z_i(\underline{x}_W . \underline{u}_i) \tag{2.1}$$

where the subscript s represents the term "simulated" or "synthetic".

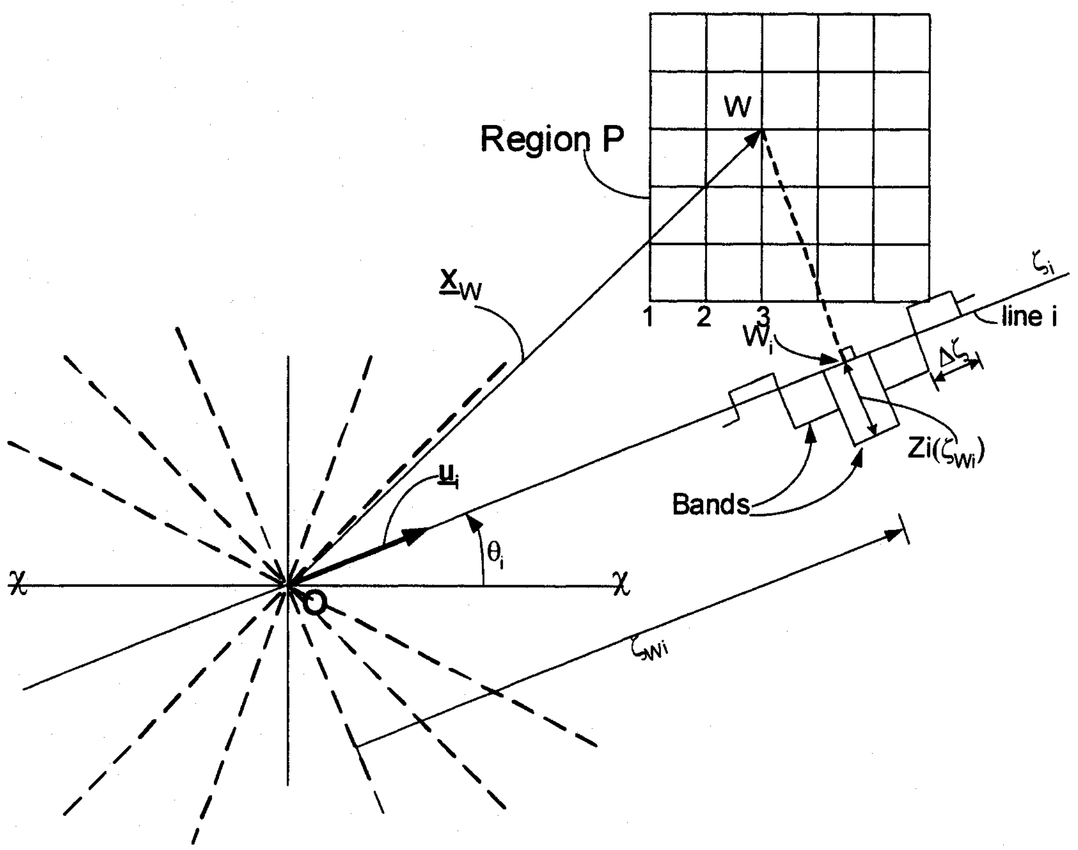


Figure 2.2 Schematic representation of the field P and the turning bands lines i (Mantoglou and Wilson, 1982)

The number of lines needed in this process essentially is infinite. However, for two-dimensional cases, Mantoglou and Wilson (1982) showed that 4 – 16 lines are sufficient. For three-dimensional cases Journel and Huijbregts (1978) showed that 15 lines are good enough to be utilized. Nonetheless, when the number of lines is small, misrepresentation related to the appearance of line-like patterns in the generated random fields and their spatial covariance might happen. This causes distortion in the generated random fields and their spatial covariance. These patterns are usually reduced when the number of lines increases. Therefore, many lines are usually needed; i.e. at least 32 and 100 lines for two-and three-dimensional, respectively (see Zhang, 2002). The details of this method can be found in Mantoglou and Wilson (1982).

Spectral Method

This method can be applied when both input and output of the processes are second-order stationary; i.e. both mean and variance of input (independent variables) and output (dependent variables) are invariant with time or space (de Marsily, 1986; Shahin et al., 1993; Gelhar, 1993; Zang, 2002). However, Zang (2002) noted that the method still can be used although the dependent variables are not stationary. Under the condition of second-order stationary, the spectral density function or spectrum of a stochastic process is the Fourier transformation of its autocovariance function. The reverse process is also applicable. The variation of hydraulic conductivity and hydraulic head values can be represented by the stochastic Fourier-Stieltjes integral representation (see de Marsily, 1986; Zang, 2002). In this method, a spatially correlated formation in the spatial domain is replaced with an uncorrelated formation in the frequency domain (Robin et al., 1993). The main steps of this method are extracted from an example given by de Marsily (1986) and they are listed below.

(1) Integrate the groundwater flow equation to obtain the mean hydraulic head gradient.
(2) Define the expected values of parameters and hydraulic heads and their fluctuation.
(3) Substitute the terms in step (2) into step (1), and take the expected value of the resulting equation to obtain an equation for perturbations.
(4) Define the complex stochastic process of the fluctuations. The complex stochastic process is the stochastic Fourier-Stieltjes integral that represents a statistically homogeneous process.
(5) Find the derivative of terms in step (4) and substitute the resulting equation into the expected values of step (3) to find equations of relationship between the Fourier amplitudes at different locations.
(6) Calculate the spectrum, expected values, variance, and covariance of head fluctuations.

Robin et al. (1993) used the spectral method to make a computer algorithm for the purpose of generating cross-correlated real random fields in a three-dimensional domain. In their work, they started with a certain power spectral density function to estimate the spectral density function directly from real data. Using the inverse Fourier Transform, they transformed the cross-correlation between the dependent and independent variables into a cross spectrum. Then the resulting cross spectrum is used to generate the random fields that show spatial correlation. They found that the computation using this algorithm is very efficient. There is also no lineation problem arise such as in the turning bands method. This algorithm can co-generate cross-correlated random fields. The details of the method are given in the paper of Robin et al. (1993).

Method of Perturbation

Sun and Yeh (1992) used the perturbation method to solve the stochastic inverse problem and analyzed the reliability of the model. In their work, they used the adjoint state method to obtain the Stochastic Partial Differential Equations, SPDE, which related transient head and perturbations of the logarithm of hydraulic conductivity. The resulting equation was used to obtain all covariance and cross-covariance matrices needed in the analysis. The steps for using this method are (Sun and Yeh, 1992; Sun, 1996, 1999)

(1) Add a value of variation to the expected value of the logarithm of hydraulic conductivity, K, and hydraulic head, H.

(2) Substitute the resulting variables into the groundwater flow equation.

(3) Take the expectation of resulting equation of step (2) to obtain a partial differential equation of the expected hydraulic head, H.

(4) Subtract equation of step (3) from equation of step (2) to obtain a stochastic partial differential equation for perturbation.

(5) Introduce a performance or objective function.

(6) Take a variation of equations of steps (4) and (5), multiply the results by the adjoint state equation, and integrate the resulting equations over the domain.

(7) Subtract the resulting equation of step (6) from the variation of equation of step (5) to obtain the functional derivative of the objective function.

(8) Solve all equations to obtain expected values of hydraulic head, and the adjoint state.

(9) Use the results to obtain the covariance and cross-covariance matrices that are used to estimate the unknown statistical parameters using the maximum likelihood estimate method.

(10) Use the resulting statistical parameters to obtain groundwater flow parameters using cokriging.

Dagan, 1997, gave a clear and step-by-step guide to do a modeling of the subsurface groundwater flow and transport in the stochastic framework and the importance of the selection of the conceptual model.

Three different methods were discussed. The Monte Carlo method is applicable to almost all groundwater flow problems. The only drawback is that the calculations have to be repeated many times. The spectral method is also a powerful method to deal with stochastic processes. Using this method the uncertainty in the prediction can be found using the statistical inference. However, this method needs the condition of stationary in both independent and dependent variables. The perturbation method, in particular the adjoint state method, does not need the stationary condition for the dependent and independent variables. This method can be used to solve many problems in groundwater flow such as sensitivity analyses, reliability estimates, design of field instrumentations, and inverse problems (see Sun, 1999). Using this method, the sensitivity matrix needed in the Gauss-Newton optimization can be avoided. As a result, the computation becomes more efficient in terms of time (see Neuman, 1980a; 1980b). Both perturbation and spectral methods need the fluctuation in the random variables to be small. Therefore, using the logarithm of hydraulic conductivity instead of hydraulic conductivity in the analysis is preferable to accommodate bigger fluctuations (see Gelhar, 1993). All methods discussed above produce comparable results. The difference between the results obtained by the last two methods, in a one dimensional case, is less than 10% if the variance of the logarithm of hydraulic conductivity is less than or equal to 1 (see de Marsily, 1986).

2.4 Stochastic Finite Element Methods in Groundwater Flow

The stochastic finite element method (SFEM) combines the finite element analysis and the stochastic methods. Most commonly, the groundwater parameters and hydraulic heads are treated as random variables. The data obtained from in situ or from laboratories are expressed in the form of probability distribution (Bear and Verruijt, 1987). The mean and covariance of hydraulic head are obtained based on the original flow equations (Gelhar, 1993). The partial differential equations are then solved using the finite element analysis to obtain hydraulic heads of the entire domain of interest. In groundwater management, this method can be used to predict the future behavior of groundwater flow.

Some researchers used the SFEM in groundwater studies. Sagar (1978) analyzed the flow through a non-uniform, heterogeneous random media using Galerkin finite element method associated with the Taylor series expansion to find the hydraulic head distribution in the study domain. He observed that the results were sensitive to the element size in the finite element discretization, the variances, and spatial correlation of parameters.

Neuman and Yakowitz (1979) used the stochastic finite element method in the solution of an inverse problem of a steady state groundwater flow to identify transmissivity of an aquifer. The method solves a group of generalized nonlinear regression problems and then selects one particular solution from this group by means of a comparative analysis of residual. In this method, it is possible to find the covariance of transmissivity estimate and the square error of the estimate of hydraulic heads. The authors found that when the errors in water level data were adequately small; this method gave a highly efficient explicit numerical scheme for solving the inverse problem in an approximate form. Moreover, the method would still be good to obtain rapidly an initial idea about the approximate position of the optimum solution when the errors were large.

Neuman (1980a) derived an adjoint finite element equation for the solution of an inverse problem of a steady state groundwater flow and identified the logarithm of transmissivity of an aquifer. His method shows that small errors in the model and in the flow rate and sink/source data have only a small effect on the estimate of the logarithm of transmissivity. Accordingly, the errors are ignored. However, the low-amplitude noise in water level had to be filtered out during the solution of the inverse problem. Otherwise, the estimate becomes unstable. He concluded that the model must be calibrated properly to obtain reasonable results.

2.5 Theory of Inverse Problems

In the forward problems, hydraulic heads can be found by solving the flow problem in a time-space domain. The solution requires as input: groundwater parameters, boundary conditions, and control variables, i.e., the pumping rate, and artificial and natural recharge rates (Kitanidis, 1997; Sun, 1999). However, in practice, it is difficult to obtain appropriate data such as the exact geometry of the flow region, hydrological parameters, boundary conditions, sink and source term obtained from field measurements. On the other hand, hydraulic heads in the observation wells can easily be measured in the field. Therefore, the observed data can be used as input data to find the groundwater parameters. This reverse way of finding the groundwater parameters is called the parameter identification or inverse solution.

In general, the inverse solution methods of groundwater flow can be categorized into two groups: (1) The methods in the first group use an error criterion equation and (2) The methods in the second group use an output error criterion (Yeh, 1986). The former is also called the direct method and the later is called the indirect method. In the direct method, one needs to solve directly a set of residual equations of computed and observed hydraulic heads at observation points to obtain an inverse solution. In this method, hydraulic heads in the entire study domain have to be known. Therefore, an interpolation of the observation data needs to be done since in practice there are only limited observation wells available. Due to error in the interpolated data, the resulting governing equation will also contain error. The equation is called the error equation and the error needs to be minimized to obtain an estimate of parameters. In the latter method, the difference between observed and calculated hydraulic heads at specified observation points is minimized. In this method, one needs to solve the inverse problem through the forward solution method. Therefore, the method is called the indirect method. It has an advantage especially when the number of observation data is limited. However, the minimization obtained is usually non-linear and often non-convex.

Parameterization is another problem of inverse solution in groundwater modeling (see Kitanidis, 1997). Parameterization is defined as a technique of the determination of the number of values a parameter can have in the study domain. The parameter values in the whole study domain then can be represented approximately by these limited number of parameter values. In a numerical groundwater flow model such as the finite element method, the study domain is discretized into many small blocks or elements. Ideally, a parameter value is assigned to each element. However, since the number of elements in the model is usually large and the number of observed data is small, then the groundwater model has too many unknown values of a parameter. This condition will cause a problem. This problem is called an over-parameterization, which can result in incorrect estimates of a parameter. Therefore, to overcome this problem, the number of unknown values of the parameter needs to be reduced or more observed values of the parameter are to be collected. The most common method to deal with this problem is to divide the study domain into zones. Each zone comprises of several elements. The value of the parameter in each zone is assumed constant. The zonation techniques in the inverse problem and sensitivity analysis in groundwater studies were used by many authors such as Newman and Yakowitz (1979), Neuman (1980a), Sykes et al. (1985), Townley an Wilson (1985), Carrera (1988), Sun and Yeh (1985, 1990a, 1990b) and Kitanidis (1997).

Stochastic approach can also be used to solve the inverse problem. In this method, both the parameters and hydraulic heads are treated as stochastic processes. The inverse solution provides the mean and covariance functions of unknown parameters (Sun, 1996).

Various researchers worked in the area of stochastic inverse problems. Hoeksema and Kitanidis (1984, 1985b), Dagan (1985), Rubin and Dagan (1987a, 1987b), Dagan and Rubin (1988) and Kitanidis (1999) used the geostatistical approach to solve the inverse problem. They estimated transmissivities of the entire domain from the measured hydraulic heads and transmissivity measurements using cokriging. Maximum likelihood was used to estimate the statistical parameters. They found that this method gives good estimates of transmissivities. Moreover, when those transmissivities were used in a numerical model, they reproduced the hydraulic head measurements quite well.

Sun and Yeh (1992) used the adjoint state equation for solving the stochastic partial differential equations as mentioned before. They found that better results were obtained when they used hydraulic head observations of all observation times simultaneously rather than using those observations sequentially (i.e. quasi-steady approach). Furthermore, a reliable stochastic inverse solution could still be obtained although the number of observations was limited.

Kitanidis (1995) used quasi-linear geostatistical approach for solving inverse problems. He estimated the log-transmissivity function using the observed values of hydraulic head and log-transmissivity at selected locations. The transmissivity was parameterized as a realization of a random field. The log-transmissivity was estimated conditional on all measurements. The method generalizes the linear approach of Kitanidis and Vomvoris (1983). By assuming that the variability of the log-conductivity or log-transmissivity was low, it was found that the estimates of parameters were stable and only slightly influenced by the grid size.

An iterative stochastic inverse method was used by Yeh et al. (1996) to estimate transmissivity and hydraulic head distribution in heterogeneous aquifers. This approach was similar to the classical cokriging technique. However, the iterative stochastic inverse method gave smaller error of the estimated transmissivity and hydraulic head fields than that obtained by the cokriging even for a high value of variance.

Kitanidis (1999) examined generalized covariance functions associated with the Laplace equation in the stochastic approach and used them in the interpolation between observed values (i.e. hydraulic heads and hydraulic conductivities). He also used the generalized covariance functions for the solution of inverse problems. He found that for natural random fields, these covariance functions were suitable. However, these covariance functions had to be adjusted for application in numerical methods.

There are some difficulties involved in the solution of inverse problems (Sun, 1999). Due to the ill-posedness, inverse methods often give non-unique solutions. Sometimes, they are also not stable. Nevertheless, those difficulties can be overcome (Carrera, 1988; Sun and Yeh, 1990a, 1990b, 1992; Kitanidis, 1995, 1999; Hoeksema and Kitanidis, 1984; Yeh et al., 1996). Carrera (1988) and Sun (1999) suggested some techniques to overcome these difficulties. Using suitable information about boundary conditions and hydraulic head measurements may eliminate the problem of non-uniqueness. The stability of results can be improved by providing upper and lower limits on the estimated parameters. Therefore, prior information on the values of parameters is essential. Moreover, as mentioned before, parameterization can also reduce the problem of instability.

Emsellem and de Marsily (1971) stated, "conductivity is a parameter with no punctual value but with an average value in a region of a given size". Therefore, they recommended that a solution that slightly varies in a certain way could be accepted.

The general steps to solve the stochastic inverse problem (SIP) are quoted from Sun and Yeh (1992) as follows.

- Use sample mean and sample variance of log K measurements as the initial estimates of statistical parameters μ_y and σ_y^2.
- Use the log K measurements only to estimate the statistical parameters μ_y, σ_y^2, and l_y through the MLE, and generate a log K field through kriging.
- Use statistical parameters obtained in the last step as the initial estimates, and use measurements of both log K and hydraulic heads simultaneously to solve the stochastic inverse problem.

2.6 Details of Forward and Inverse Solutions for Groundwater Flow Problems

Two-dimensional groundwater flow in a heterogeneous-isotropic confined aquifer is governed by the following equation (Bear, 1979)

$$S\frac{\partial \phi}{\partial t}=\frac{\partial}{\partial x}\left(Kb\frac{\partial \phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(Kb\frac{\partial \phi}{\partial y}\right)+Q \tag{2.2}$$

The solution of Eq. (2.2) requires the initial conditions (Eq. 2.2a) and boundary conditions (Eq. 2.2b) given below.

$$\phi(x,y,t)=g_0; \qquad (x,y)\in(R); \qquad t=t_0 \tag{2.2a}$$

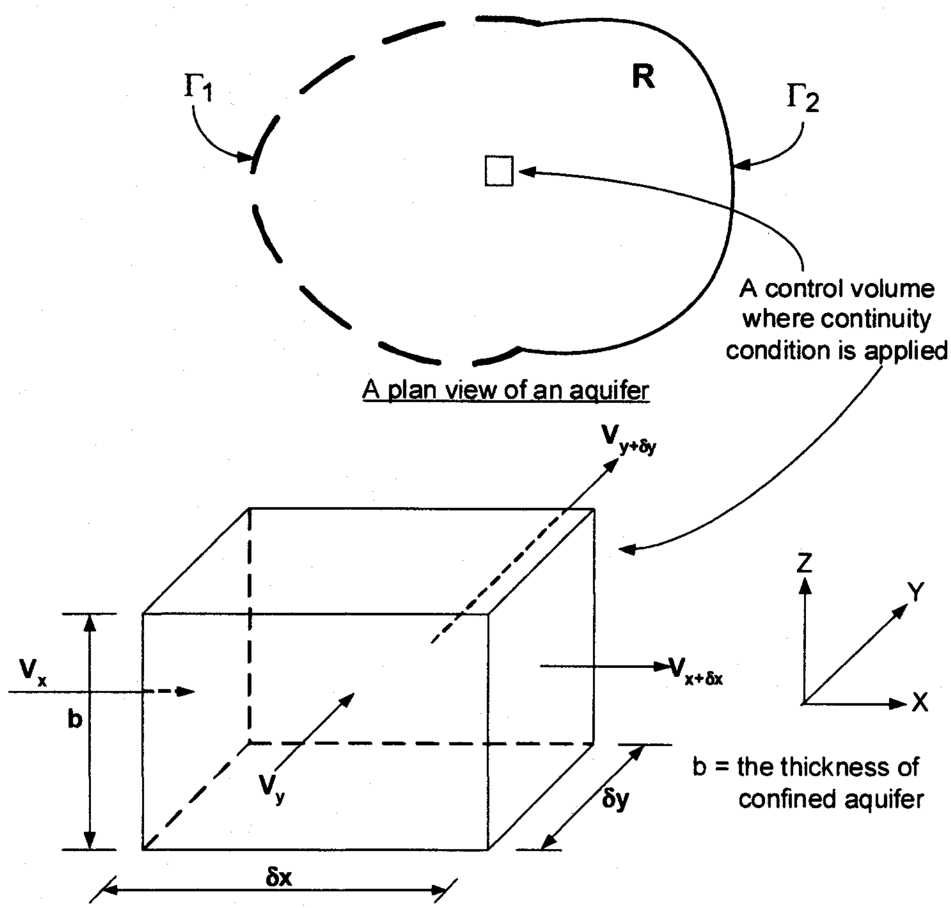
$$\phi|_{(\Gamma_1)}=g_1; \qquad \left(Kb\frac{\partial \phi}{\partial x}+Kb\frac{\partial \phi}{\partial y}\right).n\Big|_{\Gamma_2}=g_2 \tag{2.2b}$$

where

S = coefficient of storage (dimensionless)
ϕ = hydraulic head (length)
K = hydraulic conductivity (length/time)
Q = source or sink (volume/time/area)
b = thickness of the aquifer (length)
x, y = Cartesian coordinates (length)
g_0 = given functions defined on the flow region, R
g_1, g_2 = given functions defined on parts of boundary, Γ_1 and Γ_2
R = flow region
Γ_1, Γ_2= parts of boundary of the flow region, R
n = unit vector in the direction normal to Γ_2
t = time
t_0 = the initial time

The mass control volume, for which the governing equation Eq. (2.2) is based on, is presented in Figure 2.3.

In the two-dimensional groundwater flow model, the aquifer can be considered as a planar region with a thickness equal to the average thickness of the aquifer (Dagan, 1997).



V_x, V_y, and V_z are the velocity of the fluid movement in x, y, and z direction.

Figure 2.3 Mass conservation for a control volume (Bear, 1979)

2.6.1 Solution of Forward Problems

In the forward problems, unknown hydraulic heads (ϕ_i) are found by solving Eqs. (2.2), (2.2a), and (2.2b). In this case, the coefficient of storage (S), hydraulic conductivities (K_i), and the initial and boundary conditions are known. In the solution of forward problems, a vector operator U represents the governing equation of a flow problem as follows (Sun and Yeh, 1990a; Sun, 1999):

$$U(\phi, p, q; x, t) = 0 \tag{2.3}$$

with initial conditions

$$\phi = f_0 \quad \text{when} \quad t = t_0 \tag{2.3a}$$

and boundary conditions

$$\phi = f_1 \quad \text{on} \quad (\Gamma_1) \tag{2.3b}$$

$$U_{BC}(\phi, K; x, t) = f_2 \quad \text{on} \quad (\Gamma_2) \tag{2.3c}$$

where:

$$\phi = (\phi_1, \phi_2, \ldots, \phi_n)^T; \; p = (S, K_1, K_2, \ldots, K_m)^T; \; q = Q;$$
$$U = (U_1, U_2, \ldots, U_n)^T \tag{2.4}$$

t = time
x = spatial variables
U_{BC} = a vector operator representing flux boundary conditions
ϕ_i = hydraulic heads
K_i = hydraulic conductivities

The subscripts n and m denote the number of observation of hydraulic heads and hydraulic conductivities, respectively, and the superscript T is the transpose operator. Equation (2.2) has to be solved using the initial and boundary conditions to determine hydraulic head values.

2.6.2 Solution of Inverse Problems

In inverse problems the unknown hydraulic conductivities (K_i) or maybe the unknown initial and boundary conditions are found by providing continuous or discrete measurements of hydraulic heads, ϕ_i, (Sun and Yeh, 1990a).

In the inverse problems, the following parameters have to be found.

$$K^* \in A_d \quad \text{such that} \quad \phi^*(K) = z \qquad \text{at} \quad O_b \tag{2.5}$$

where

K^* = estimates of hydraulic conductivity
$\phi^*(K)$ = calculated hydraulic heads when the estimates of K are employed
A_d = a proper set of unknown parameters
O_b = a set of observation wells and observation times
z = observations of hydraulic heads

Observation errors will always be there; as a result, it is impossible to obtain an exact solution to Eq. (2.5); therefore, an approximate solution by minimization procedure is followed as explained below.

$$\text{to find } K^* \in A_d \text{ such that } \Omega(K^*) = \min \Omega(K) \quad ; \quad K \in A_d \tag{2.6a}$$

where

$$\Omega(K) = (\Omega_1(K), \Omega_2(K), \ldots, \Omega_n(K))^T \tag{2.6b}$$

$\Omega_i(K)(i = 1,2,\ldots,n) =$ a performance criterion for measuring the residual between the model output and observations of hydraulic heads ϕ_i when K is used as the model parameter.

Using the least squares criterion, $\Omega_i(K)$ can be estimated as

$$\Omega_i(K) = \left\| \phi_i(K) - z_i \right\|_{L_2}^{2} \qquad i = 1,2,\ldots,n \tag{2.7}$$

where

$\phi(K) - z_i$ = a vector that represents the residuals between the model output of ϕ_i and its observations at set Ob

$\left\| \bullet \right\|_{L_2}$ = the L_2 norm (Sun, 1999)

The problem defined by Eq. (2.7) is called a vector optimization problem (VOP) or multi-objective problem (see Sun and Yeh, 1990a). Taking benefit of a priori knowledge for estimated parameters, problem (2.6b) can be modified as

$$\hat{\Omega}(K) = \left(\Omega_1(K), \ldots, \Omega_n(K), \Omega_{n+1}(K), \ldots, \Omega_{n+m}(K)\right)^T \tag{2.8}$$

where $\Omega_{n+j}(K)$ (j = 1,2,…,m) is a performance criterion for measuring the residual between parameter K_j and its a priori estimation.

Using the least square criterion, this performance criterion can be modified as

$$\Omega_{n+j}(K) = \left\| K_j - K_j^0 \right\|_{L_2}^{2} \tag{2.9}$$

where K^0_j is a priori estimation of parameter K_j. The solution of inverse problem becomes

$$\text{to find } K^* \in A_d \text{ such that } \hat{\Omega}(K^*) = \min \hat{\Omega}(K); \qquad K \in A_d \tag{2.10}$$

The weighting method can be used to obtain the solutions of the VOP (2.10) in terms of optimal solution of their appropriate scalar optimization problem (SOP). A scalar objective can be defined as

$$w(K) = \sum_{i=1}^{n+m} w_i \Omega_i(K) \tag{2.11}$$

where w = $(w_1, w_2, \ldots, w_{n+m})^T$ is a weighting coefficient vector with all its components positive. Using the following SOP, the solution of Eq. (2.11) can be obtained.

$$w\left(\hat{K}\right) = min\, w(K); \qquad K \in A_d \tag{2.12}$$

where $\hat{K}$ is the estimated value of K.

There are three categories for solving the SOP (2.12), i.e. Gauss-Newton, gradient search, and direct search methods (Sun and Yeh, 1990a). Following Sun and Yeh (1990a, 1992), in this thesis the Gauss-Newton method that has broadly used in the groundwater flow study will be employed. In this method, in every iteration of the non-linear least square minimization, it is essential to compute the total sensitivity matrix as follows:

$$JB_{w} = \begin{bmatrix} \left[\frac{\partial \phi_1}{\partial K_1}\right] & \left[\frac{\partial \phi_2}{\partial K_1}\right] & \cdots & \left[\frac{\partial \phi_n}{\partial K_1}\right] \\ \left[\frac{\partial \phi_1}{\partial K_2}\right] & \left[\frac{\partial \phi_2}{\partial K_2}\right] & \cdots & \left[\frac{\partial \phi_n}{\partial K_2}\right] \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \left[\frac{\partial \phi_1}{\partial K_m}\right] & \left[\frac{\partial \phi_2}{\partial K_m}\right] & \cdots & \left[\frac{\partial \phi_n}{\partial K_m}\right] \end{bmatrix} \tag{2.13}$$

To determine the Jacobian or sensitivity matrix Eq. (2.13), there are three methods (Yeh, 1986), i.e. the influence coefficient method, the sensitivity coefficient method, and the variational or adjoint state method. Following Sun and Yeh (1990a, 1990b, 1992), the adjoint state method will be used in this study.

2.7 Available Programs

As mentioned before, the solution of a mathematical model for a complex and large domain needs a computer program. There are a few commercially available computer-programs to solve the inverse problem of groundwater flow. Some of them will be reviewed below.

(1) MODFLOWP (http://water.usgs.gov/software/Modflowp.html)

MODFLOWP is a computer program for solving inverse problems developed by United State Geological Survey (USGS). This program uses the finite difference technique to solve the governing equations. It can handle both three-dimensional transient and steady state groundwater flow problems. A nonlinear regression method is used in the program. The input data include prior estimates of parameter values, observed hydraulic heads at any observation time, and observed inflow and outflow along head boundaries. Besides providing the model parameters, statistics for the parameter estimates and the model output are also included. By utilizing these statistics, the reliability of the resulting model can be calculated and changes necessary for constructing a better model can be suggested.

In the calibration procedure, the program minimizes a weighted least-squares objective function by using either the modified Gauss-Newton method or a conjugate-direction method. This program can be used to estimate the following input parameters that are needed for the forward solution of a groundwater problem.

- Transmissivity and coefficient of storage of confined aquifers
- Hydraulic conductivity and specific yield of unconfined aquifers
- Vertical leakage
- Vertical anisotropy
- Horizontal anisotropy
- Hydraulic conductance of rivers, stream flow-routing and head boundaries.
- Area recharge rates
- Maximum evapotranspiration
- Pumping rates

(2) PEST (http://www.sspa.com/pest/)

PEST is a general program for parameter estimation. It uses a non-linear parameter estimation method called the Gauss-Marquardt-Levenberg method. This program can be used to estimate model parameters of groundwater flow and mass transport both at saturated and unsaturated zone of aquifers. Furthermore, it can also be used to estimate parameters of surface-water flow problems. The program is capable of estimating hundreds of parameters based on thousands of measurements of complex aquifer systems. Moreover, it can perform sensitivity analysis and gives the statistics of the resulting parameters.

(3) GEOPACK (http://ggsd.com/index.htm)

GEOPACK is a geostatistical program for analyzing the spatial variability of one or more random variables. The program is developed by the EPA/USA. This program can do linear parameter estimation and its variance in two-dimensional domain using the ordinary kriging and cokriging estimators. Moreover, it has non-linear estimators like the disjunctive kriging and disjunctive cokriging. Basic statistic analyses that are provided by this program include mean, median, variance, standard deviation, skew, and kurtosis and max/min values. Furthermore, linear and polynomial regression and some statistical tests such as the Kolmogorov-Smirnov test for distribution, and calculation of some percentile of a data set are also provided. Program can determine sample semivariogram, cross-semivariogram or semivariogram for combined random functions for a two-dimensional spatially dependent random variable.

(4) SOILPARA (http://www.scisoftware.com)

SOILPARA is parameter estimator software for determining hydraulic properties of groundwater flow and mass transport in unsaturated and saturated soils. The technique used in the program is based on statistical pore/particle size distribution. This program can be used to estimate hydraulic parameters in the Van Genuchten fundamental model for variably saturated soils. It can estimate up to 7 parameters. Marquardt method is used for estimating the parameters.

(5) UCODE (http://water.usgs.gov/software/ucode.html)

UCODE (Poeter and Hill, 1998) is a computer program for universal inverse modeling. It is designed mainly for groundwater modeling. The program provides statistical results that can be used

(a) to diagnose insufficient data and to recognize the unidentified parameters
(b) to find identified parameter values
(c) to evaluate the model capability of the actual processes
(d) to quantify the probable uncertainty of simulated values

The program uses a non-linear regression method. The minimization of weighted square objective function of the model with respect to the parameter values is done by the modified Gauss-Newton method.

(6) GROUNDWATER VISTAS (STOCHASTIC MODFLOW)
(http://www.groundwater-vistas.com/html/groundwater_vistas_details.html)

GROUNDWATER VISTAS is a program for modeling stochastic groundwater flow and transport. In doing the stochastic analysis, the Monte Carlo simulation method is utilized. This program is capable of doing a geostatistical simulation using the kriging technique; therefore, "it provides a single, smooth, deterministic estimate of what the field may look like" (Manual of Groundwater Vistas). This program can simulate up to 50 different uncertain parameters for each stochastic simulation. Distribution types that can be simulated include (1) normal, (2) log-normal, (3) uniform, (4) log-uniform, and (5) triangulár. However, this program only deals with steady state problems.

CHAPTER 3

THEORETICAL DEVELOPMENT FOR THE SOLUTION OF STOCHASTIC INVERSE PROBLEM IN GROUNDWATER FLOW

3.1 Stochastic Partial Differential Equations

To obtain a solution for a stochastic inverse problem in groundwater flow, the governing equation, Eq. (2.2), needs to be solved. This can be achieved by using a direct method or an indirect method. The input data required for the solution consist of observed hydraulic conductivities, hydraulic head measurements, storage coefficients, initial and boundary conditions, and the amount of discharge and/or recharge in the aquifer. In this study, hydraulic conductivity and hydraulic head values are considered random variables. They are represented by their expected values plus their perturbations. The expected values and the perturbation terms for both variables are substituted into equation Eq. (2.2). As a result, two stochastic partial differential equations (SPDE) are obtained. They are (1) an SPDE for the expected heads and (2) an SPDE for the perturbations in hydraulic conductivities and hydraulic heads. These SPDE are then solved to obtain expected hydraulic heads and adjoint state values. The definition of the adjoint state function is given later in this chapter and a detailed explanation is provided in Appendix A using equations from (A15) to (A21). These values are then used to calculate the covariance matrices of hydraulic heads at different times and the cross-covariance matrices between hydraulic conductivities and hydraulic heads in the study domain. The resulting covariance and cross-covariance matrices are used in the MLE analysis to obtain the statistical parameters of the groundwater flow problem. Finally, the cokriging method is used to estimate the distribution of hydraulic conductivity in the study domain by utilizing the resulting statistical parameters. The details of the method are written in the following sections.

Following Freeze (1975), Neuman (1980a), Hoeksema and Kitanidis (1985a), and Sun and Yeh (1992), it is assumed that the coefficient of storage is constant in the entire aquifer and Y = log K is normally distributed. It is also common to assume normal distribution for Y = ln K (Dagan, 1997). More importantly, this phenomenon has been observed in the field by Robin et al. (1991). The simulation can be simplified by representing K as a constant mean value of Y plus a perturbation based on the covariance (autocovariance) or variogram. One of the assumptions underlying the use of the autocovariance function or variogram is that the autocovariance depends on the distance separating measurement points, but does not depend on the locations of the points. Moreover, for certain form of covariance, the entire parameter framework can be represented by three statistical parameters: the mean (μ_Y), variance (σ_Y^2), and correlation scale (l_Y). In addition, Neuman (1980a) points out that the estimates of the logarithm of hydraulic conductivity are always positive when the logarithm of hydraulic conductivity is used instead of K. In this thesis, Y = ln K is used.

Following Hoeksema and Kitanidis (1985a), Dagan (1985), Wagner and Gorelick (1989), and Sun and Yeh (1992); it is assumed that the random field Y is characterized by a constant mean and an isotropic, exponential covariance as follows

$$E[Y] = \mu_Y \tag{3.1}$$

$$Cov_{YY}(x_i, x_j) = \sigma_Y^2 \, exp\left(-\frac{d_{ij}}{l_Y}\right) \tag{3.2}$$

where

$E[Y]$ = the expected value of logarithm of hydraulic conductivity
σ_Y^2 = the variance of the logarithm of hydraulic conductivity
l_Y = the correlation scale of the logarithm of hydraulic conductivity

d_{ij} = the distance between points x_i and x_j
μ_Y = the mean of the logarithm of hydraulic conductivity
x_i, x_j = the locations of points in the study domain that are separated by a distance of d_{ij}

Inherent in the development and use of Eqs. (3.1) and (3.2) are the condition of second-order stationary and the assumption of ergodicity of the stochastic process. The second order stationary condition is commonly used in the geostatistical estimation procedures (Isaaks and Srivastava, 1989). It means that the mean and variance are space independent. A stochastic process is ergodic if its ensemble statistics can be represented by its spatial statistics. In a hydrological context ergodicity must be assumed because only one realization can be obtained from field measurements (see Robin, 2002). Covariance of Eq. (3.2) is one of the most common covariance used in the groundwater flow studies (Kitanidis, 1997).

In the stochastic analysis, when the first-order analysis such as the perturbation or spectral method of analysis is employed (see Kitanidis, 1997), the random variables Y and ϕ can be expressed as follows.

$$Y = F + f; \qquad \phi = H + h \tag{3.3}$$

where

F = the expected value of Y, E[Y]
H = the expected value of ϕ, E[ϕ]
f = the variation of Y about the mean value
h = the variation of ϕ about the mean value

Substituting Eq. (3.3) into Eq. (2.2) yields

$$S\frac{\partial(H+h)}{\partial t} = \frac{\partial}{\partial x}\left(e^{F+f} b\frac{\partial(H+h)}{\partial x}\right) + \frac{\partial}{\partial y}\left(e^{F+f} b\frac{\partial(H+h)}{\partial y}\right) + Q \tag{3.4}$$

After some derivations and rearrangements (given in detail in Appendix A), the following equation is obtained.

$$e^F\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)\right]+e^F\left[\frac{\partial}{\partial y}\left(b\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right]$$
$$+be^F\left(\frac{\partial f}{\partial x}\frac{\partial H}{\partial x}\right)+be^F\left(\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}\right)+Q-fQ-S\frac{\partial H}{\partial t} \qquad (3.5)$$
$$-S\frac{\partial h}{\partial t}+fS\frac{\partial H}{\partial t}=0$$

In derivation of Eq. (3.5), the following terms are ignored because of the smallness of the terms.

$$\frac{\partial h\partial f}{\partial x\partial x},\ \frac{\partial h\partial f}{\partial y\partial y},\ \text{and}\ f\frac{\partial h}{\partial t} \qquad (3.6)$$

Moreover (see the Appendix A), if the variation in f is small, then exp(-f) can be approximated by (1-f) (Gutjahr and Gelhar, 1981; Dagan, 1982a; Mizell et al., 1982; Hoeksema and Kitanidis, 1985b; and Sun and Yeh, 1992).

Other assumptions are that the storage coefficient, S, and thickness of the aquifer, b, are deterministic parameters and their values are known.

Taking expectation of Eq. (3.5), a stochastic partial differential equation, SPDE, for the expected H can be obtained as follows

$$S\frac{\partial H}{\partial t}=e^F\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial H}{\partial y}\right)\right]+Q \qquad (3.7)$$

Subtracting Eq. (3.7) from Eq. (3.5) an SPDE for perturbations f and h is obtained as follows.

$$S\frac{\partial h}{\partial t}=e^{F}\left[\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right]$$
$$+be^{F}\left(\frac{\partial f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}\right)+f\left(S\frac{\partial H}{\partial t}-Q\right) \tag{3.8}$$

Assuming f and h to be unknown and S to be known, the variational equation of Eq. (3.8) becomes

$$S\frac{\partial \delta h}{\partial t}=e^{F}\left[\frac{\partial}{\partial x}\left(b\frac{\partial \delta h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial \delta h}{\partial y}\right)\right]$$
$$+be^{F}\left(\frac{\partial \delta f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial \delta f}{\partial y}\frac{\partial H}{\partial y}\right)+\delta f\left(S\frac{\partial H}{\partial t}-Q\right) \tag{3.9}$$

The initial and boundary conditions are

$$\delta h\big|_{t=0}=0; \qquad (x,y)\in(R) \tag{3.9a}$$

$$\delta h\big|_{\Gamma_1}=0; \qquad e^{F}\left(\frac{\partial \delta h}{\partial x}+\frac{\partial \delta h}{\partial y}\right)\cdot n\big|_{\Gamma_2}=0 \tag{3.9b}$$

where Γ_1 and Γ_2 are boundaries of the flow region.

In the adjoint state method, an arbitrary function ψ is introduced into Eq. (3.9). ψ is called the adjoint state or importance function. Sykes et al. (1985) defined it as a function that "represents the change in the value of the performance measure caused by a unit volume influx of water at any point x in the domain".

Following Thomson and Sykes (1986), Sun and Yeh (1992), and Kitanidis (1997), the objective or "influence" function of an inverse solution can be chosen as

$$\Omega(h,f)=\int_{0}^{T}\int_{R}G(h,f;x,t)dRdt \tag{3.10}$$

where T is a given time and G is a user-chosen function.

The variation of performance function Ω is

$$\delta\Omega=\int_{0}^{T}\int_{R}\left(\frac{\partial G}{\partial h}\delta h+\frac{\partial G}{\partial f}\delta f\right)dRdt \tag{3.11}$$

After some derivations and application of Green's first identity to the Eqs. (3.9) and (3.11), the following equations can be obtained (see Appendix A).

$$\frac{\partial G}{\partial h}=S\frac{\partial \psi}{\partial t}+e^{F}\left[\frac{\partial}{\partial x}\left(b\frac{\partial \psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial \psi}{\partial y}\right)\right] \tag{3.12}$$

$$\frac{\partial \Omega}{\partial f}=\int_{0}^{T}\int_{R}\left\{\frac{\partial G}{\partial f}+e^{F}b\left[\frac{\partial \psi}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial \psi}{\partial y}\frac{\partial H}{\partial y}\right]\right\}dRdt \tag{3.13}$$

Equation (3.12) is called the adjoint problem of the main problem of Eq. (2.2). Equation (3.13) is the functional derivatives of the objective function of Eq. (3.10) (Neuman, 1980b; Sun and Yeh, 1985, 1990a, 1992).

In Eq. (3.12) the following conditions can be assumed

$$\psi(x,y,t)=0;(x,y)\in(R);t=t_0 \tag{3.14a}$$

$$\psi\big|_{\Gamma_1}=0; \qquad e^{F}\left(\frac{\partial \psi}{\partial x}+\frac{\partial \psi}{\partial y}\right)\cdot n\big|_{\Gamma_2}=0 \tag{3.14b}$$

Derivation of the equations can be found in Sun and Yeh (1992); Sun (1999), and in Appendix A.

Solution of Eq. (3.13) can be obtained by a numerical integration after a function G in Eq. (3.10) is chosen (Neuman, 1980a, 1980b; Thomson and Sykes, 1986; Sun and Yeh, 1992). Expected hydraulic heads, H, can be obtained by solving Eq. (3.7) and the adjoint state, ψ, can be determined by solving Eq. (3.12). It needs to be noted that the adjoint states are calculated backward in time; i.e. start from t = T and move toward t = 0 (Neuman, 1980b; Thomson and Sykes, 1986; and Neupauer and Wilson, 2001).

The derived adjoint equations by employing the variational method are a set of partial differential equations in the continuous form. In this approach, the derivative of the governing equation does not need any approximations; therefore, the resulting equations are most relevant and most precise. Moreover, existing numerical algorithms can be used to solve the resulting adjoint equation precisely (Yeh and Sun, 1990).

3.2 Determination of Covariance Matrices

Following Thomson and Sykes (1986), and Sun and Yeh (1992), function G in Eq. (3.10) can be chosen as

$$G(x,t) = h(x,t)\delta(x - x_l)\delta(t - t_p) \tag{3.15}$$

where

x = any point in the study domain
t = any time used in the calculation
x_l = the location of an observation well
t_p = an observation time
$\delta(\cdot)$ = the Dirac δ function

To calculate the functional derivative for any node i, Eq. (3.13) has to be modified as shown in the following equation

$$\frac{\partial h(x_l, t_p)}{\partial f_i} = \int_0^T \int_{R_i} \left\{ e^F b \left[\frac{\partial \psi}{\partial x}\frac{\partial H}{\partial x} + \frac{\partial \psi}{\partial y}\frac{\partial H}{\partial y} \right] \right\} dR dt \tag{3.16}$$

where (R_i) is the exclusive sub domain of node i (Neuman and Yakowitz, 1979; Neuman, 1980a, 1980b; Sun and Yeh, 1985).

All elements of the following (L x N) Jacobian, $JB_D(t_p)$, can be calculated using Eq. (3.16).

$$JB_D(t_p) = \left[\frac{\partial h_D(t_p)}{\partial f} \right] \tag{3.17}$$

where L is the number of observation wells, N is the number of nodes, $h_D(t_p)$ is the observed hydraulic head perturbation vector at time t_p, and f is a vector of the perturbations of the logarithm of K for all nodes (Sun and Yeh, 1992).

The (L x L) covariance matrix of observed hydraulic heads at time t_p can be calculated as a first order approximation by employing the Jacobian, $JB_D(t_p)$, as follows (Sun and Yeh, 1992).

$$Q_{D,\phi\phi}(t_p, t_p) = E\left[h_D(t_p) h_D^T(t_p)\right] = JB_D(t_p) E\left[ff^T\right] JB_D^T(t_p) \tag{3.18}$$

The superscript T denotes the transpose of a vector or matrix and the letter Q is used in general to denote the covariance matrix.

The (L x L) covariance matrix between hydraulic head observations at observation time t_{p1} and t_{p2} can be obtained by

$$Q_{D,\phi\phi}(t_{p1}, t_{p2}) = E\left[h_D(t_{p1}) h_D^T(t_{p2})\right] = JB_D(t_{p1}) E\left[ff^T\right] JB_D^T(t_{p2}) \tag{3.19}$$

and the (L x M) cross-covariance matrix related to measured hydraulic heads and values of the logarithm of K can be calculated by

$$Q_{D,\phi Y}(t_p) = E\left[h_D(t_p) f_D^T\right] = JB_D(t_p) E\left[f f_D^T\right] \tag{3.20}$$

M is the number of observation of Y. Matrix $E[ff^T]$ is the covariance matrix of Y at all nodes; therefore, the size of this matrix is (N x N). This matrix can be determined by the given covariance structure Eq. (3.2). Matrix $E[ff^T{}_D]$ is the covariance matrix between Y measurements and Y of all nodes and it has a size of (N x M). This matrix is a sub-matrix of $E[ff^T]$.

3.3 Estimation of Unknown Statistical Parameters

Following Kitanidis and Vomvoris (1983), and Sun and Yeh (1992), the statistical parameters, which are shown in Eqs. (3.1) and (3.2) can be calculated using the maximum likelihood estimate (MLE) as follows.

$$LG(z|\theta) = \frac{LT}{2} ln(2\pi) + \frac{1}{2} ln|Q_D| + \frac{1}{2}(z-\mu)^T Q_D (z-\mu) \tag{3.21}$$

where

θ = Statistical parameter vector. The elements of θ are μ_Y, σ_Y^2, and l_Y, the values of which are not known. l_y is the correlation scale.

z = the measurement vector

LT = the total number of measurements

Q_D = the measurements covariance matrix

μ = the mean vector of measurements

Both Q_D and μ are functions of unknown statistical parameters.

In the transient flow problem, hydraulic head observations at different observation time have to be known. Those data can be utilized to identify the parameter vector θ using two methods as follows (Sun and Yeh, 1992):

1. Identify vector θ_p ($p = 1, 2, \ldots, P$) at each observation time t_p with the hydraulic head observation for that certain time interval only using MLE successively. Taking average value of θ_p of entire time, the θ estimate can be obtained (Dagan and Rubin, 1988). The measurement covariance matrix for observation time t_p can be calculated by

$$Q_D = \begin{bmatrix} Q_{D,\phi\phi}(t_p, t_p) & Q_{D,\phi Y}(t_p) \\ Q_{D,\phi Y}(t_p) & Q_{D,YY} \end{bmatrix} \tag{3.22}$$

In Eq. (3.22), $Q_{D,\phi\phi}$ and $Q_{D,\phi Y}$ are calculated using Eqs. (3.18) and (3.20) respectively. $Q_{D,YY}$ is the Y measurement covariance matrix that can be obtained by using Eq. (3.2). LT in Eq. (3.21) is equal to (L+ M).

2. Identify vector θ_p ($p = 1, 2, \ldots P$) by using hydraulic head and hydraulic conductivity observations at all measurement times simultaneously. The measurement covariance matrix for all observation times can be calculated by

$$Q_D = \begin{bmatrix} Q_{D,\phi\phi}(t_1, t_1) & \cdots & Q_{D,\phi\phi}(t_1, t_p) & Q_{D,\phi Y}(t_1) \\ \cdot & \cdots & \cdot & \cdot \\ \cdot & \cdots & \cdot & \cdot \\ Q_{D,\phi\phi}(t_p, t_1) & \cdots & Q_{D,\phi\phi}(t_p, t_p) & Q_{D,\phi Y}(t_p) \\ Q_{D,\phi Y}(t_1) & \cdots & Q_{D,\phi Y}(t_p) & Q_{D,YY} \end{bmatrix} \tag{3.23}$$

where $Q_{D,\phi\phi}(t_p, t_p)$, $Q_{D,\phi\phi}(t_{p1}, t_{p2})$, and $Q_{D,\phi Y}(t_p)$ can be obtained from Eqs. (3.18), (3.19), and (3.20), respectively. LT in Eq. (3.21) is equal to [(L x P) + M] and the size of matrix Q_D is [(L x P) + M] x [(L x P) + M].

3.4 Estimation of the logarithm of K field

The logarithm of K field can be determined using a geostatistical approach by either the Gauss conditional mean or cokriging method (Hoeksema and Kitanidis, 1985b; Dagan, 1985; de Marsily, 1986; Rubin and Dagan, 1987a; Dagan and Rubin, 1988). In determining the logarithm of K field, measurements of both hydraulic head and the logarithm of K are used. In the Gaussian conditional mean method, the estimate of parameters can be obtained by determining the statistical moments of Y, i.e., the expected value and the covariance of Y; conditional on the measured values of Y_i ($i = 1,\ldots,M$) and H_j ($j = 1,\ldots,L$). It is assumed that both the conditional pdf of Y and the unconditional joint pdf Y and H to be Gaussian. The coefficients that relate Y and H and their relative position in the domain can be obtained by solving simultaneously a linear system of equations for which the unconditional second moment is needed for the solution. Then for every point in the study domain, the value of Y* can be obtained by adding the expected value of Y by its residuals. The residuals are resulted from summation and multiplication of the resulting coefficients with the differences between the measured values of Y and H at each point with their mean values. The cokriging method is similar to the Gaussian conditional mean method regarding the linear relationship between Y and its residuals and H. However, in the Gaussian conditional mean method the expected values of Y and H are assumed to be known exactly that leads to the underestimation of the error variance. On the other hand, in the cokriging method, the mean values of both H and Y are assumed to be completely unknown. As a result the cokriging method is superior to the Gaussian conditional mean method since the resulting estimation variance is smaller (Hoeksema and Kitanidis, 1985b). Moreover, the cokriging method is the best linear unbiased estimation method since in this approach the equation involved in the estimation procedure is a linear equation and the estimation error is forced to be zero with the coefficients used in the process defined such that the variance of the estimation error is minimized (Isaaks and Srivastava, 1989; Kitanidis, 1997). However, Hoeksema and Kitanidis (1985b) found that both methods give reliable estimates of the logarithm of transmissivity field.

The cokriging method is used in this research to obtain the estimate of logarithm of K in the entire domain. In this method, all measured hydraulic heads at different time and measured logarithm of hydraulic conductivities are used simultaneously in the following equation.

$$\hat{Y}_0 = \sum_{p=1}^{P} \sum_{l=1}^{L} \xi_{l,p} \left(\phi_{l,p} - H_{l,p}\right) + \sum_{m=1}^{M} \lambda_m Y_m \tag{3.24}$$

where $\hat{Y}$ is the logarithm of K estimate.

Cokriging coefficients λ_m and $\xi_{i,p}$ can be obtained by solving simultaneously the following equations for each point in the study domain

$$\sum_{p=1}^{P} \sum_{l=1}^{L} \xi_{l,p}, Cov\left[\phi(x_i, t_j), \phi(x_l, t_p)\right] + \sum_{m=1}^{M} \lambda_m Cov\left[\phi(x_i, t_j), Y(x_m)\right] + \upsilon_l$$
$$= Cov\left[\phi(x_i, t_j), Y(x_0)\right] \quad i = 1, 2, \ldots, L; j = 1, 2, \ldots, P \tag{3.25a}$$

$$\sum_{p=1}^{P} \sum_{l=1}^{L} \xi_{l,p} Cov\left[Y(x_i), \phi(x_l, t_p)\right] + \sum_{m=1}^{M} \lambda_m Cov\left[Y(x_m), Y(x_0)\right]$$
$$+ \upsilon_2 = Cov\left[Y(x_0), Y(x_i)\right] \; ; \; i = 1, 2, \ldots, M \tag{3.25b}$$

$$\sum_{m=1}^{M} \lambda_m = 1 \tag{3.25c}$$

$$\sum_{p=1}^{P} \sum_{l=1}^{L} \xi_{l,p} = 0 \tag{3.25d}$$

where

$Cov[\phi(x_i, t_j)\ \phi((x_l, t_p)]$	= the covariance between the hydraulic head observation at point x_i and time t_j and the hydraulic head observation at point x_l and time t_p
$Cov[\phi(x_i, t_j)\ Y(x_m)]$	= the cross-covariance between the observed hydraulic head at point x_i and time t_j and the logarithm of measured K value at point x_m
$Cov[Y(x_0)\ Y(x_m)]$	= the covariance between the logarithms of measured K values at point x_0 and point x_m

The number of equations in Eq. (3.25) is [M + (L x P) + 2] in which there are [M + (L x P)] cokriging coefficients λ_m and ξ_i, and two other coefficients v_1 and v_2 that are named the Lagrange multipliers. The coefficients λ_m and ξ_i are the weighted coefficients that allow one to estimate unknown parameter values at different locations and the Lagrange multipliers, v_1 and v_2, are coefficients that help to convert a constrained minimization problem into an unconstrained one (see Isaaks and Srivastava, 1989).

The Eqs. (3.24) and (3.25) are called the cokriging system (see Isaaks and Srivastava, 1989). In the matrix form, they can be written as follows.

$$[CA]\{\beta\} = \{DA\} \tag{3.26}$$

where

$$[CA] = \begin{bmatrix} \bar{C}_{\phi_{ii}\phi_{ll},t_j t_k} & \cdots & \bar{C}_{\phi_{ii}\phi_{ll},t_j t_k} & \bar{C}_{\phi Y} & 1 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \bar{C}_{\phi_{ii}\phi_{ll},t_j t_k} & \cdots & \bar{C}_{\phi_{ii}\phi_{ll},t_j t_k} & \bar{C}_{\phi Y} & 1 & 0 \\ \bar{C}_{Y\phi} & \cdots & \bar{C}_{Y\phi} & \bar{C}_{Y_m Y_0} & 0 & 1 \\ 1 & \cdots & 1 & 0 & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 & 0 \end{bmatrix} \tag{3.27}$$

The dimension of matrix [CA] is {(MxL)+2} x {(MxL)+2}.

$$\{DA\} = \begin{Bmatrix} \bar{C}_{\phi_{x_i} Y_0} \\ . \\ . \\ \bar{C}_{\phi_{x_i} Y_0} \\ \bar{C}_{Y_0 Y_i} \\ 0 \\ 1 \end{Bmatrix} \tag{3.28}$$

The dimension of matrix {DA} is (M x L) + 2.

$$\{\beta\} = \begin{Bmatrix} \xi_{l,p} \\ . \\ . \\ \xi_{l,p} \\ \lambda_m \\ 0 \\ 1 \end{Bmatrix} \tag{3.29}$$

The dimension of matrix {β} is (M x L) + 2.

Therefore, the cokriging coefficients can be obtained using the following equation.

$$\{\beta\} = [CA]^{-1}.\{DA\} \tag{3.30}$$

where $[CA]^{-1}$ is the inverse of matrix $[CA]$.

$\bar{C}_{\phi_i \phi_l, t_j t_k}$ in Eq. (3.26) is Cov[ϕ(x_i, t_j) ϕ((x_l, t_p)] in Eq. (3.25) and can be calculated using Eqs. (3.18) and (3.19). $\bar{C}_{\phi Y}$ in Eq. (3.26) is Cov[ϕ(x_i, t_j) Y(x_m)] in Eq. (3.25) and can be calculated using Eq. (3.20) while $\bar{C}_{Y\phi}$ is the transpose of $\bar{C}_{\phi Y}$. $\bar{C}_{Y_m Y_0}$ in Eq. (3.26) is Cov[Y(x_0) Y(x_i)] in Eq. (3.25) and can be calculated using Eq. (3.2).

The variance of cokriging estimate can be determined by (Isaaks and Srivastava, 1989)

$$Var\left[\hat{Y}_0 - Y_0^*\right] = \sigma_Y^2 - \sum_{m=1}^{M} \lambda_m Cov\left[Y(x_m), Y(x_0)\right]$$
$$- \sum_{p=1}^{P} \sum_{l=1}^{L} \xi_{l,p} Cov\left[\phi(x_l, t_p), Y(x_0)\right] - \upsilon_2 \qquad (3.31)$$

After calculating the $\hat{Y}$ estimate, its value will be compared with the true values of Y^*. Those values can be compared using L_2 -norm as follows (Sun and Yeh, 1992):

$$CY = \left\| Y^* - \hat{Y} \right\|_{L2} = \left[\frac{1}{M} \sum_{m=1}^{M} \left(Y_m^* - \hat{Y}_m \right)^2 \right]^{1/2} \qquad (3.32)$$

3.5 Steps for Solving the Stochastic Inverse Problem

1. Solve Eq. (3.7) to obtain expected hydraulic head H.
2. Solve Eq. (3.12) to obtain the adjoint state ψ.
3. Calculate the functional derivative in Eq. (3.13) by a numerical integration and use the results to obtain the Jacobian of Eq. (3.17).
4. Calculate the covariance and cross-covariance matrices of Eqs. (3.18), (3.19), (3.20), and (3.22) or (3.23).
5. Estimate the unknown statistical parameters μ_y, σ_y, and l_y using MLE by means of Eq. (3.21).
6. Use cokriging to estimate the logarithm of K field by means of Eq. (3.24).

CHAPTER 4

STOCHASTIC FINITE ELEMENT FORMULATION AND COMPUTER PROGRAMMING

4.1 Stochastic Finite Element Formulation

In the finite element analysis using the Galerkin method, an approximate or trial solution of the expected hydraulic head, $\hat{H}$, can be expressed as a summation of products of nodal hydraulic heads, H_L, and the weighted averages in terms of basis functions $\zeta_L(x,y)$ (Wang and Anderson, 1982); i.e.

$$\hat{H}(x,y) = \sum_{L=1}^{NNODE} H_L \zeta_L(x,y) \tag{4.1}$$

where subscript L is nodal number and NNODE is the total number of nodal points in the problem domain. In order to solve Eq. (3.7) for the expected head, H, both sides of this equation are multiplied by the basis function first. Then, integration is performed over the entire domain. After some derivations and the application of Green's first identity, one can obtain the following matrix equation.

$$[A]\{H\}^{t+\Delta t} = \{M\} + [D]\{H\}^t \tag{4.2}$$

where

$$[A] = e^F b[C] + [D] \tag{4.3}$$

[A] is an L x L matrix.

$$[D]=\frac{1}{\Delta t}[P] \tag{4.4}$$

[D] is an L x L matrix that contains the amount of storage defined in the L x L matrix [P]. Matrix [C] is also an L x L matrix. For each nodal point of an element, matrix [C] is calculated by the following equations.

$$C_{L,i}^{el} = A^{e}\left(\frac{\partial \zeta_L^{el}}{\partial x}\frac{\partial \zeta_i^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y}\frac{\partial \zeta_i^{el}}{\partial y}\right) \tag{4.5a}$$

$$C_{L,j}^{el} = A^{el}\left(\frac{\partial \zeta_L^{el}}{\partial x}\frac{\partial \zeta_j^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y}\frac{\partial \zeta_j^{e}}{\partial y}\right) \tag{4.5b}$$

$$C_{L,k}^{el} = A^{el}\left(\frac{\partial \zeta_L^{el}}{\partial x}\frac{\partial \zeta_k^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y}\frac{\partial \zeta_k^{el}}{\partial y}\right) \tag{4.5c}$$

In the global sense, matrix [C] is a summation of $C_{L,m}^{el}$. Matrix [C] becomes

$$[C]_{L,m} = \sum_{el} C_{L,m}^{el}\text{, for all L and m where L = i, j, k and m = i, j, k} \tag{4.5d}$$

The amount of storage is expressed in the matrix [P] in Eq. (4.4). For each nodal point in an element, matrix [P] is calculated by the following equations.

$$P_{L,i}^{el} = S\iint_{el} \zeta_i^{el}\zeta_L^{el}\,dxdy \tag{4.6a}$$

$$P_{L,j}^{el} = S\iint_{el} \zeta_j^e \zeta_L^e dxdy \tag{4.6b}$$

$$P_{L,k}^{el} = S\iint_{el} \zeta_k^{el} \zeta_L^{el} dxdy \tag{4.6c}$$

In the global coordinate system, matrix [P] is expressed as follows.

$$[P]_{L,m} = \sum_{el} P_{L,m}^{el} \text{ , for all L and m where L = i, j, k and m = i, j, k} \tag{4.6d}$$

The amount of recharge and/or discharge in a nodal point in an element is calculated by the equations given below.

$$M_i^{el} = \iint_{el} Q\zeta_i^{el}(x,y)dxdy = QA^{el}/3 \tag{4.7a}$$

$$M_j^{el} = \iint_{el} Q\zeta_j^{el}(x,y)dxdy = QA^{el}/3 \tag{4.7b}$$

$$M_k^{el} = \iint_{el} Q\zeta_k^{el}(x,y)dxdy = QA^{el}/3 \tag{4.7c}$$

The recharge-discharge matrix {M} in the global coordinate system is obtained by the following equation.

$$\{M\}_L = \sum_{el} M_L^{el} \text{ , for all L where L = i, j, or k} \tag{4.7d}$$

where

L = number of the nodal points in an element
$\zeta(x,y)$ = the basis function
e^F = the exponent of the expected logarithm of hydraulic conductivity
A^{el} = the area of elements

Δt = time steps
Superscript el = the element under consideration
Subscripts i, j, k = the nodal points of triangular elements

The other symbols are similar to those used in Chapter 3. In this thesis, triangular elements as illustrated in Figure 4.1 are used.

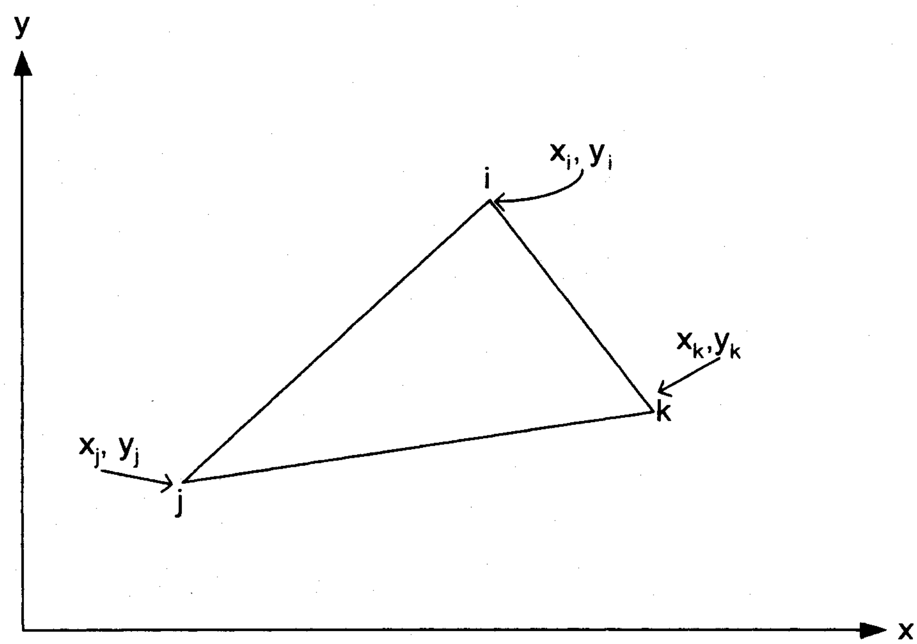


Figure 4.1 A typical triangular element for the finite element calculation. Nodal numbers i, j, k are indexed counter clockwise direction (from Wang and Anderson, 1982)

Similar to the previous section, an approximate or trial solution of the adjoint state, $\hat{\psi}$, can be expressed as a series of summations which is a product of nodal adjoint states, ψ_L, and the weighted average in term of basis functions $\zeta_L(x,y)$; i.e.

$$\hat{\psi}(x,y) = \sum_{L=1}^{NNODE} \psi_L \zeta_L(x,y) \tag{4.8}$$

The methodology used in the derivation of Eq. (4.2) can be applied to Eq. (3.12) to obtain the finite element equations in matrix form as follows.

$$[A]\{\psi\}^{t+\Delta t} = [D]\{\psi\}^{t} + \{E\} \tag{4.9}$$

where

$$[A] = e^{F} b[C] + [D] \tag{4.10}$$

[A] is an L x L matrix.

The column matrix {E} is a matrix that is used to calculate the gradient of function G. The value of this gradient in each node in an element can be calculated using the following equations.

$$E_{L,i}^{el} = \iint_{el} \zeta_i^{el} \zeta_L^{el} \frac{\partial G_i}{\partial h} dxdy \tag{4.11a}$$

$$E_{L,j}^{el} = \iint_{el} \zeta_j^{el} \zeta_L^{el} \frac{\partial G_j}{\partial h} dxdy \tag{4.11b}$$

$$E_{L,k}^{el} = \iint_{el} \zeta_k^{el} \zeta_L^{el} \frac{\partial G_k}{\partial h} dxdy \tag{4.11c}$$

In the global coordinate system, the gradient of function G, {E}, is given below.

$$\{E\}_{L,m} = \sum_{el} E_{L,m}^{el} \text{, for all L and m where L = i, j, or k and m = i, j, k} \tag{4.11d}$$

Matrices [D] and [C] have been defined before in Eqs. (4.4) and (4.5).

Considering Eqs. (4.1) and (4.8), Neuman (1980b) implies that

$$\frac{\partial \Omega}{\partial f} = \frac{\partial \Omega}{\partial f_i} \zeta_i \tag{4.12}$$

Utilizing Eq. (4.12), Eq. (3.16) can be expressed as

$$\frac{\partial h(x_l,t_p)}{\partial f_i}=\int_0^T\int_{R_i}\left\{e^F b\left[\frac{\partial\psi}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial\psi}{\partial y}\frac{\partial H}{\partial y}\right]\right\}\zeta_i(x,y)dRdt \tag{4.13}$$

After the expected head, H, and the adjoint state, Ψ, were obtained by solving Eqs. (4.2) and (4.9), the results can be substituted into Eq. (4.13) and the resulting equation becomes (see Neuman, 1980b)

$$\frac{\partial h(x_l,t_p)}{\partial f_i}=e^F b\sum_{n=1}^{NNODE}\sum_{m=1}^{NNODE}B_{inm}\sum_p\int_p^{t_{p+1}}\psi_n H_m dt \tag{4.14}$$

where

$$B_{inm}=\int_R\nabla\zeta_n\cdot\nabla\zeta_m\cdot\zeta_i(x,y)dR \tag{4.15}$$

where n and m are nodal numbers, and i is the number of parameter zones.

The third summation in Eq. (4.14) must be held over all time steps for every node in the study domain. Therefore, each number of the expected head, H, and the adjoint state,Ψ, needed for the calculation is equal to $\left[MxNx\left(\frac{T}{\Delta t}\right)\right]$ where T and Δt are the total simulation time and the time interval, respectively. Since the time interval is smaller than 0.05 unit time, which makes the solution stable, the number of calculated heads, H, and the adjoint states,Ψ, becomes large. The derivations of the finite element equation are given in Appendix B.

4.2 Computer Programming

Computer programs are developed to solve the stochastic partial differential equations of inverse problems related to groundwater flow. Three different computer programs are developed as listed in Section 1.3. The first computer program is developed using FORTRAN language and the last two programs in the list are developed using MATLAB. The overall program is named STOCHINV. The flowcharts of these programs are presented in Appendix D.

CHAPTER 5

VERIFICATION AND VALIDATION OF THE FINITE ELEMENT PROGRAM

To check whether the program works correctly and represents the real behavior of aquifers, it needs to be verified and validated.

5.1 Verification

Verification of a program is achieved by making sure that the equations used in every step of a mathematical/numerical model are coded correctly. A verified program gives results exactly the same as a correct solution of equations obtained by other means. There are closed-form solutions to some simple engineering problems. They can be used for verification purposes. However, all newly written programs need to be verified for complex and large problems. Konikow and Bredehoef (1992) stated that the analytical solutions introduces simplicity in geometry, uniform properties, and idealized boundary and initial conditions. In the numerical solutions these simplicities are not needed. Therefore, the results of these two types of solution methods cannot always be compared directly.

5.1.1 Verification of Deterministic Inverse Program

In this research, the deterministic inverse computer program is verified by solving a hypothetical groundwater problem. The verification process has two steps.

1. In the first step, a forward analysis is performed to obtain the distribution of hydraulic heads in the entire aquifer at various time intervals. In the forward

analysis, hydraulic conductivity values are provided as input. A number of wells are used to observe the hydraulic head changes at various time intervals.

2. In the second step, an inverse analysis is used. Contrary to the forward analysis, the hydraulic conductivity values are the unknowns in the inverse analysis. The hydraulic heads at the observation wells as calculated in the forward analysis are specified as input. The program finds the optimum values of hydraulic conductivity values by minimizing the difference between the calculated and observed hydraulic heads. Once the differences are minimized, the hydraulic conductivities calculated by the inverse analysis are compared well with those used in the forward analysis.

The program for the solution of the deterministic inverse problem is a modification of the one given in Sun (1999). This program deals with inverse problem using the Gauss-Newton method. Input data include geometry and geological information such as x and y coordinates of each node in the problem domain, initial and boundary conditions, aquifer thickness, and aquifer parameters. Moreover, some control numbers such as weighting coefficients used in the Gauss-Newton and Levenberg-Marquard methods are also required as input. The explanation of these methods can be found, for example, in the book of Fletcher (1999).

As shown in Fig. 5.1a, the hypothetical model makes use of a confined aquifer. The horizontal area, $\overline{ABCD}$, which is shown in Fig. 5.1b, is a plan view of the aquifer. The area, $\overline{ABCD}$, is 600 m wide and 1200 m long. The hypothetical model is taken from the book of Sun (1999). This area is divided into 40 triangular elements and 30 nodes. Boundary conditions are as follows. The hydraulic head along the side $\overline{AB}$ is constant with a value of 100.00 m. The other three sides, i.e., sides $\overline{BC}$, $\overline{CD}$ and $\overline{DA}$ have boundary conditions of no groundwater flow across the boundary. The problem domain is divided into two zones; i.e. Zone 1 is from element number 1 to 24 and Zone 2 is from element number 25 to 40, with different hydraulic conductivities and coefficients of storage. It is assumed that the aquifer has a constant thickness of 50 m. The values of the coefficient of storage are assumed 0.001 and 0.002 for Zone 1 and Zone 2, respectively. The initial hydraulic head at all nodes is 100.00 m. In order to make the problem transient, pumping is performed at one of the wells at nodal point 23 with a discharge of 4000 m^3/day. There is a recharge well at nodal point 8 with the flow rate of 500 m^3/day. Four observation wells located at nodal points 8, 14, 17, and 23 are used to observe the change in hydraulic heads. At those wells, the hydraulic heads are calculated at various time intervals.

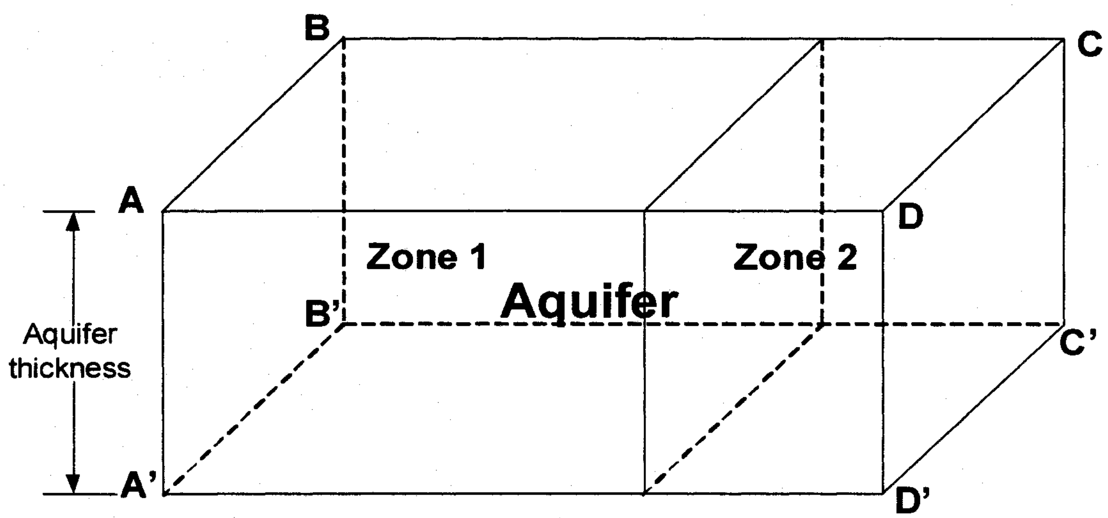


Figure 5.1a Three-dimensional view of the aquifer

ABB′A′ = Constant head
ADD′A′ = No flow perpendicular to this surface
DCC′D′ = No flow perpendicular to this surface
BCC′B′ = No flow perpendicular to this surface
Note: The aquifer is confined between the top surface (ABCD) and the bottom surface (A′B′C′D′).

5.1.1.1 Results and Discussion

The forward analysis is performed with specified hydraulic conductivity values. The specified hydraulic conductivities are 5 m/day and 10 m/day for Zone 1 and Zone 2, respectively. The hydraulic heads in the entire aquifer are calculated. The hydraulic heads at observation wells at various time intervals are recorded. The hydraulic heads at all nodes after 50 days and the hydraulic heads at the observation wells at all time intervals are shown in Tables 5.1 and 5.2, respectively. The hydraulic heads in the entire aquifer after 50 days is shown in Fig. 5.2.

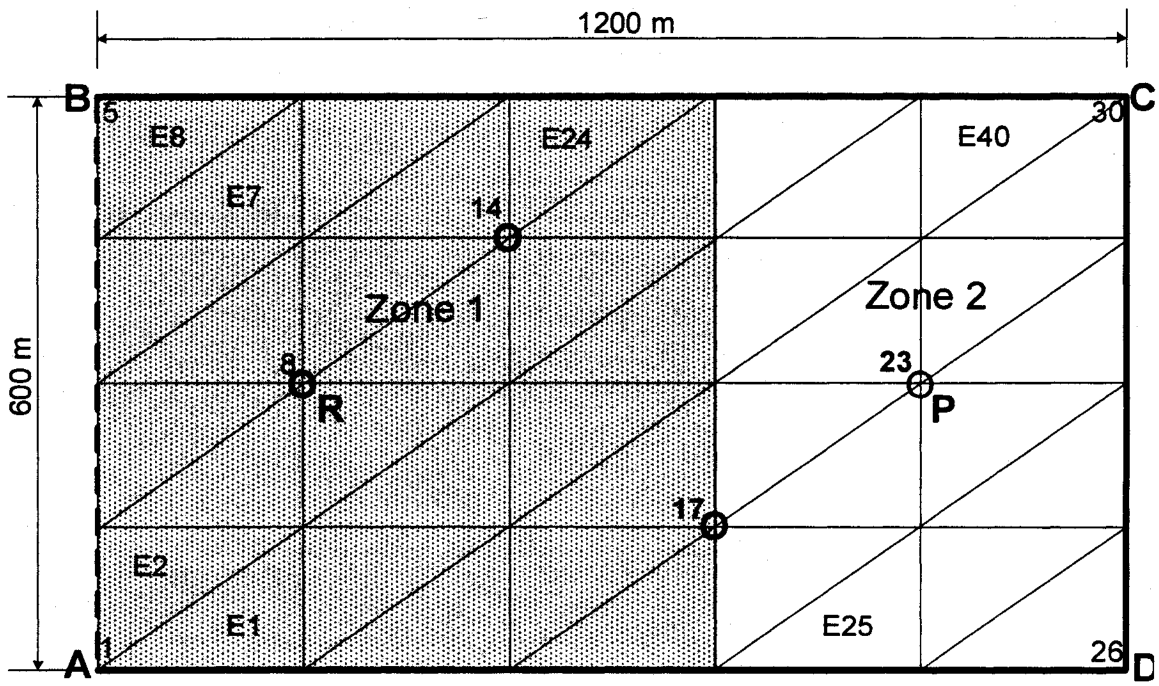


Figure 5.1b Plan view of the hypothetical problem (from Sun, 1999)

R = A recharge well
O = An observation well
P = A pumping well
1, 5,... = Node numbers
E1, E2,... = Element numbers
S1 = 0.001 S2 = 0.002
K1 = 5 m/d K2 = 10 m/d

Note:
Initial total hydraulic heads at all nodes = 100.00 m
Constant hydraulic head at side $\overline{AB}$ = 100.00 m
Sides $\overline{BC}$, $\overline{CD}$, $\overline{DA}$ = No flow across the boundaries
Q at node number 8 = 500 m^3/d (recharge)
Q at node number 23 = -4000 m^3/d (discharge)

Subsequently, the inverse solution procedure is followed. The hydraulic heads at the observation wells calculated in the forward analysis are used as input in the inverse analysis. Initial estimates of hydraulic conductivities and the upper and lower bounds of hydraulic conductivities in two zones are given as input as well as the geometry of the system. In practice, these values are estimated from prior knowledge. Through the forward analysis, the values of hydraulic heads at all nodal points are calculated. Then the calculated hydraulic heads in the inverse solution are compared with the hydraulic heads recorded in the forward solution. Both values have to be comparable within specified limits. The Gauss-Newton method algorithm is utilized to minimize the objective function. The values of hydraulic conductivity in the inverse analysis are modified automatically until the resulting hydraulic heads fit to the observed hydraulic heads; i.e. the difference between calculated and observed hydraulic heads is minimized.

Table 5.1 Hydraulic heads at nodes at observation time: 50 days

Node	Head (m)	Node	Head (m)	Node	Head (m)	Node	Head (m)	Node	Head (m)
1	100	7	95.08	13	88.86	19	82.45	25	79.92
2	100	8	95.79	14	88.81	20	82.57	26	79.45
3	100	9	95.08	15	88.78	21	79.92	27	79.27
4	100	10	94.88	16	82.57	22	79.49	28	78.91
5	100	11	88.78	17	82.45	23	77.99	29	79.27
6	94.88	12	88.81	18	82.22	24	79.49	30	79.45

Table 5.2 Hydraulic heads at observation wells

Time	Node #8	Node #14	Node #17	Node #23
(day)	(m)	(m)	(m)	(m)
0.10	101.10	100.04	99.91	97.80
0.50	101.37	99.82	98.49	95.82
1.00	100.83	98.59	96.44	93.43
2.00	99.73	96.44	93.32	89.97
5.00	97.58	92.27	87.38	83.43
10.00	96.29	89.76	83.81	79.49
20.00	95.86	88.93	82.63	78.19
30.00	95.82	88.85	82.51	78.06
40.00	95.80	88.82	82.47	78.01
50.00	95.79	88.91	82.45	77.99

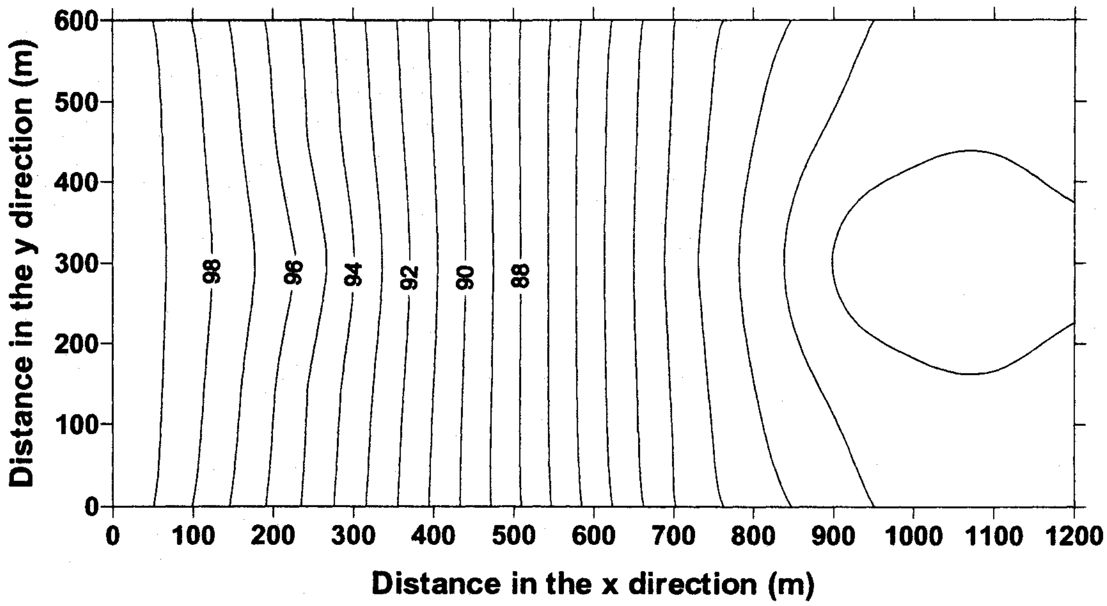


Figure 5.2 Contour lines of hydraulic heads in the study domain at time = 50 days

Calculated results can be seen in Table 5.3. It is shown that the observed and calculated hydraulic heads at all observation wells for all time intervals fit quite well when the values of hydraulic conductivity for Zone 1 and Zone 2 are 5 m/day and 10 m/day, respectively. Therefore, it can be said that the program is verified for this particular problem. The verification process will be continued with some other types of problems. Verification problems with various boundary conditions, increased number of zones with different hydraulic conductivities and coefficient of storage, and various discharge and recharge values will be considered in the future.

Table 5.3: The comparison between observation and calculated hydraulic heads

Results of the calibration

K1 = 5 m/day S1 = 0.001

K2 = 10 m/day S2 = 0.002

The injection well (node# 8)					Obs. well no.2 (Node# 14)					Obs. well no.3 (Node# 17)					The pumping well (Node# 23)				
No	Time (day)	Obs1 (m)	Cal1 (m)	D %	No	Time (day)	Obs2 (m)	Cal2 (m)	D %	No	Time (day)	Obs3 (m)	Cal3 (m)	D %	No	Time (day)	Obs4 (m)	Cal4 (m)	D %
1	0.1	101.10	101.10	0.00	1	0.1	100.04	100.04	0.00	1	0.1	99.91	99.91	0.00	1	0.1	97.80	97.80	0.00
2	0.5	101.37	101.37	0.00	2	0.5	99.82	99.82	0.00	2	0.5	98.49	98.49	0.00	2	0.5	95.82	95.81	0.01
3	1	100.83	100.83	0.00	3	1	98.59	98.59	0.00	3	1	96.44	96.44	0.00	3	1	93.43	93.43	0.00
4	2	99.73	99.73	0.00	4	2	96.44	96.44	0.00	4	2	93.32	93.32	0.00	4	2	89.97	89.97	0.00
5	5	97.58	97.58	0.00	5	5	92.27	92.27	0.00	5	5	87.38	87.38	0.00	5	5	83.43	83.42	0.01
6	10	96.29	96.29	0.00	6	10	89.76	89.76	0.00	6	10	83.81	83.81	0.00	6	10	79.49	79.49	0.00
7	20	95.86	95.86	0.00	7	20	88.93	88.93	0.00	7	20	82.63	82.63	0.00	7	20	78.19	78.19	0.00
8	30	95.82	95.82	0.00	8	30	88.85	88.85	0.00	8	30	82.51	82.51	0.00	8	30	78.06	78.06	0.00
9	40	95.80	95.80	0.00	9	40	88.82	88.82	0.00	9	40	82.47	82.47	0.00	9	40	78.01	78.01	0.00
10	50	95.79	95.79	0.00	10	50	88.81	88.81	0.00	10	50	82.45	82.45	0.00	10	50	77.99	77.99	0.00

5.1.2 Verification of Stochastic Analysis Program

Two comparisons are made for the verification of the stochastic finite element program. In real-life field problems, the "true" value of hydraulic conductivity distribution is not known. Therefore, for verification purposes, it is decided to create a hypothetical model with built-in randomness in the values of hydraulic conductivity and hydraulic head in an aquifer. Once the hypothetical model is created, the stochastic analysis program is used to estimate the distribution of hydraulic conductivity in the aquifer. The results of the stochastic analysis program and the hypothetical model are compared to verify the stochastic analysis program.

The steps for creating the hypothetical model are as follows:

1. Consider a confined aquifer that has one discharge well.
2. Select a mean value for the logarithm of hydraulic conductivity for the aquifer.
3. Develop a collection of random numbers using a random number generator. The generated random numbers must follow a normal distribution with zero mean and specified variance. They represent the variation around the mean value of the logarithm of hydraulic conductivity for the aquifer.
4. Add randomly one of the generated random numbers to the mean value of logarithm of hydraulic conductivity for each node in the aquifer. The resulting numbers are used to draw contour lines of the logarithm of hydraulic conductivity in the aquifer. The contour lines are drawn by utilizing a plotting program called, SURFER, which utilizes kriging method for interpolation. Note that the logarithms of hydraulic conductivity values are converted to hydraulic conductivities for the purpose of achieving clarity in plotting.
5. Create a finite element mesh for the aquifer. Divide the aquifer into several zones, with each zone comprised of several finite elements. The contour map discussed in step 4 should also be divided into zones identical to the zones of the finite element mesh. The need for zonation is explained in Section 2.5. Note that in the verification of the program, the zonation is chosen based on a priori information about the aquifer such as the pattern of the "true" values of hydraulic conductivity, the direction of the groundwater flow, and the location of observation wells.

6. Pick randomly one position from one of the zones in the contour map. Assign this logarithm of hydraulic conductivity value to all the elements in the same zone of the finite element mesh. Continue the process until all elements of the finite element zones are assigned the logarithm of hydraulic conductivity values. Obtain a forward solution to calculate the distribution of hydraulic heads in the aquifer.
7. Repeat step 6 a sufficient number of times to obtain a statistical distribution of hydraulic heads at every node of the finite element mesh. Several nodes in the finite element mesh can be chosen as the locations of observation wells. During the finite element analysis of forward solution, record the changes in the hydraulic head values at these nodes (observation wells) as a function of time.

Once the hypothetical model is created, by using the steps described above, the values of hydraulic heads in the observation wells of the hypothetical model are used as input for the stochastic inverse analysis. The distribution of the resulting hydraulic conductivities calculated by the stochastic inverse analysis program, STOCHINV, must have the same pattern of hydraulic conductivity distribution as that of the hypothetical model.

5.1.2.1 Verification of stochastic analysis program – Case 1

The verification is achieved by making a comparison between the distribution of hydraulic conductivity of the hypothetical model and the distribution of hydraulic conductivity predicted by the stochastic inverse analysis program. The first thing to do is to create a hypothetical model. For this purpose, a confined aquifer is chosen. Figure 5.3 shows a plan view of the aquifer. The thickness of the aquifer is assumed to be 60 metres everywhere. On the boundaries of the domain, the sections labeled as $\overline{BC}$ and $\overline{EF}$ are assigned constant head values of 80 and 70 metres, respectively. The sections labeled as $\overline{CDE}$ and $\overline{FAB}$ are chosen as no-flow boundaries. Figure 5.4 shows the assumed initial hydraulic heads everywhere in the aquifer. The model domain is discretized into 144 elements using 91 nodes. In order to have a transient flow conditions, a pumping well (PW) is introduced at node 46 with a discharge value of 4000 m^3/day. There are five observation wells located at nodes 20, 31, 46, 65, and 82, which will be used to observe the hydraulic heads at different times during the calculation as will be discussed later. The pumping well at node 46 is also considered to be an observation well. The aquifer is assumed to have 5 different parameter zones in which each zone has a different value of storage coefficient (S). The storage coefficients of all zones are given in Table 5.4.

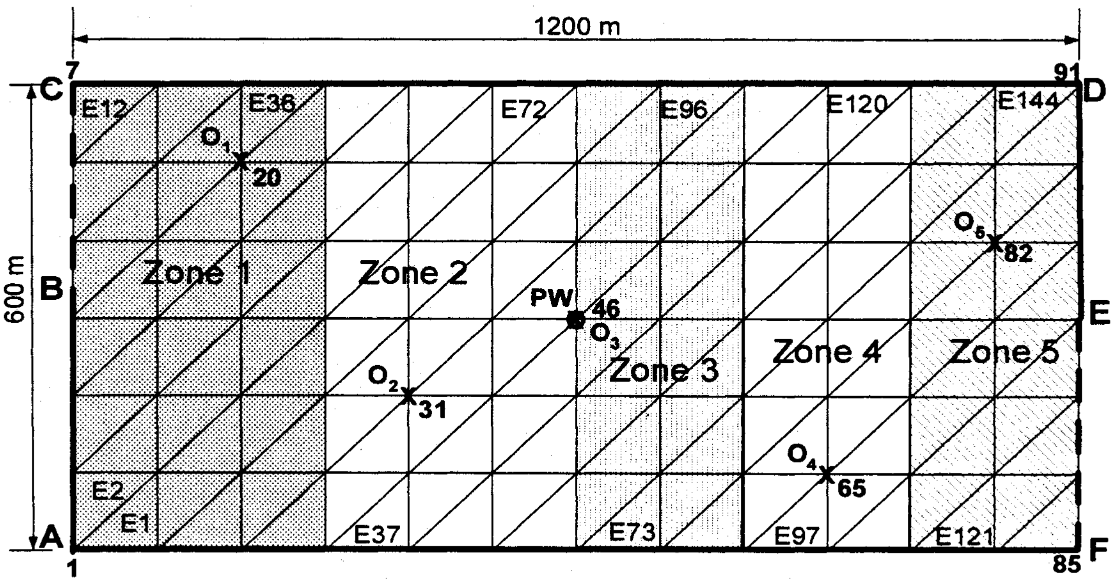


Figure 5.3 Plan view of the hypothetical problem used for the verification of the stochastic analysis program – Case 1

Legend:	Note:
O = An observation well	Constant hydraulic head at side $\overline{BC}$ = 80.00 m
PW = A pumping well	Constant hydraulic head at side $\overline{EF}$ = 70.00 m
1, 2,... = Node numbers	Sides $\overline{CDE}$ and $\overline{FAB}$ = No flow across the boundaries
E1, E2,... = Element numbers	Q at node number 46 = -4000 m^3/d (discharge)

The realization of the logarithm of hydraulic conductivity (K*) in the entire aquifer is obtained using a random number generator with $\mu_Y = 3.5$ and $\sigma_Y = 0.15$ and seed number = 1226. Altogether, 2000 random numbers were generated. From these 2000 numbers, 91 numbers were chosen randomly to draw contour lines of hydraulic conductivity using the plotting program SURFER. The contour lines are presented in Figure 5.5. These values are referred to as the "true values" of the hydraulic conductivity. It is noted that all plots and tables of hydraulic conductivity presented in this thesis are in the natural arithmetic scale. However, in the calculations, the logarithmic values of hydraulic conductivity are used.

Table 5.4 The values of storage coefficients in different zones used for the verification of the stochastic analysis program – Case 1

Zone Number	Element Number	S
1	E1 – E36	0.0002
2	E37 – E72	0.0001
3	E73 – E96	0.0002
4	E97 – E 120	0.0003
5	E121 – E144	0.0004

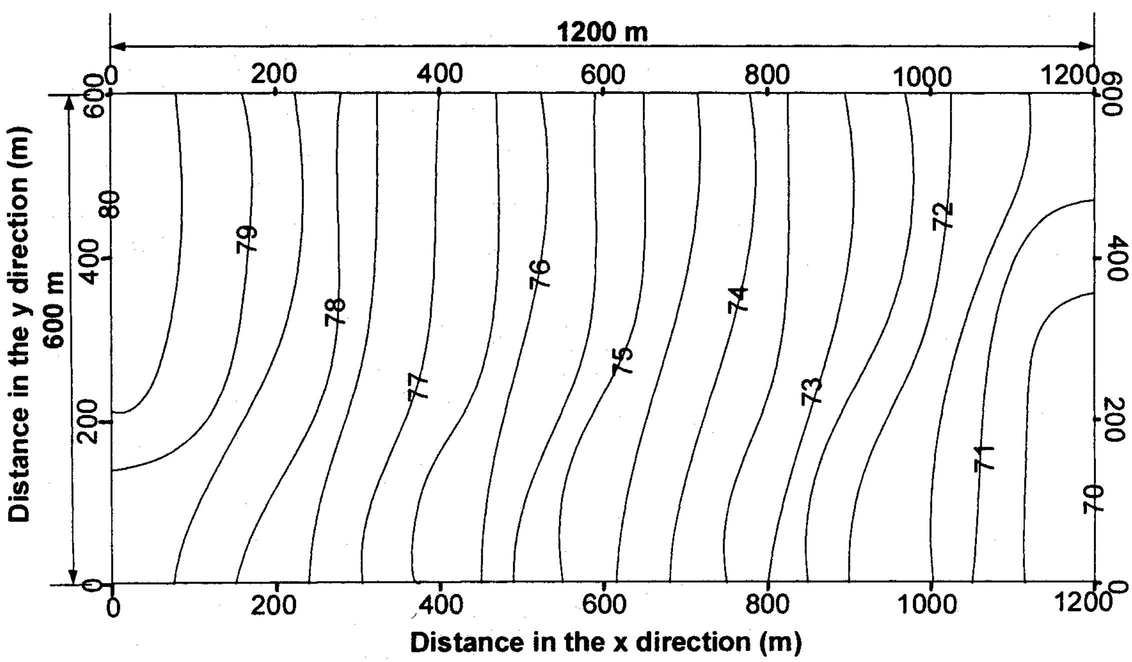


Figure 5.4 The initial conditions of hydraulic heads (metres). This figure is used in the verification of the stochastic analysis program – Case 1

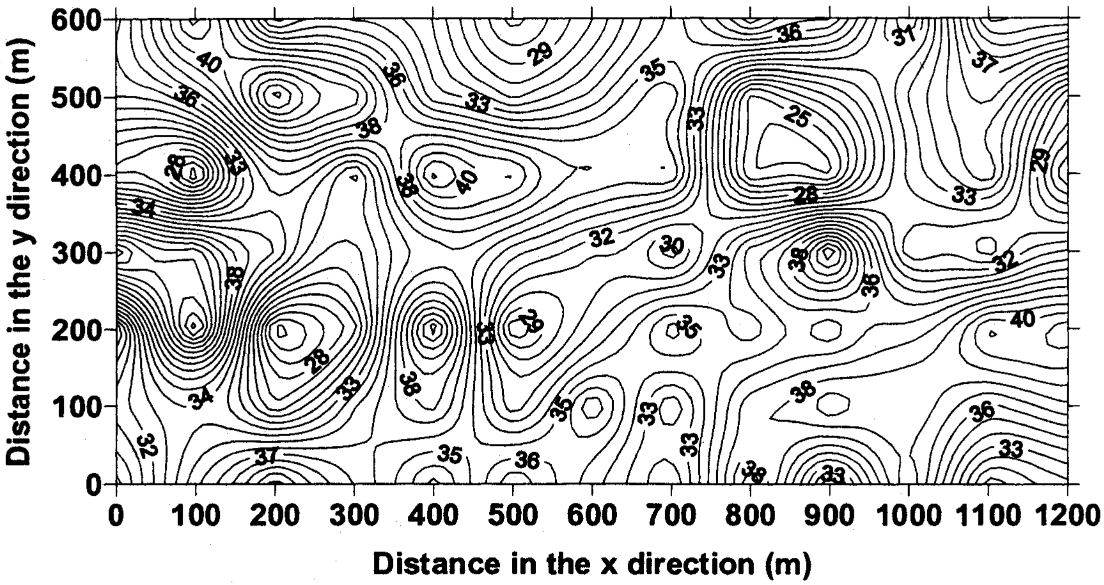


Figure 5.5 The "true" hydraulic conductivity distribution (m/d). This figure is used in the verification of the stochastic analysis program – Case 1

After the distribution of the hydraulic conductivity is plotted, the problem is solved many times using the forward solution method (for example NN times) to obtain the hydraulic head distribution in the aquifer at different times. In this part of the calculations to develop the hypothetical model, the initial conditions, boundary conditions, storage coefficients, the amount of discharge, and the logarithm of hydraulic conductivity values for different zones are used as input. The forward solution is carried out many times. Each time the forward solution was performed, the logarithm of hydraulic conductivity values assigned as input to different parameter zones were taken randomly from the corresponding zones of the plot of contour lines of hydraulic conductivities shown in Figure 5.5. Each forward solution gave the hydraulic heads everywhere in the aquifer, including the nodes representing the observation wells, as a function of time. The hydraulic head data at the observation wells are collected at different observation times in all forward solutions. Therefore, at the end of forward solutions, there are NN x NT number of hydraulic heads. NT is the number of the observation times. In each observation well, at each observation time, the value of hydraulic head is the average value of the hydraulic heads obtained from the overall NN forward solutions at the same observation time. The average values of hydraulic heads are given in Table 5.5. They are assumed to be the measured hydraulic heads at these observation wells in the hypothetical model. The last row in Table 5.5 gives the observed hydraulic conductivity values at the observation wells. With this information, the description of the hypothetical model becomes complete.

Table 5.5 "Measured" hydraulic conductivities and hydraulic heads at observation wells used for the verification of the stochastic analysis program – Case 1

	Hydraulic heads (m)				
Node number	20	31	46	65	82
Time (day)					
0.05	77.85	75.67	73.53	72.17	71.44
0.1	77.81	75.60	73.45	72.12	71.40
0.2	77.80	75.57	73.42	72.10	71.38
0.5	77.79	75.55	73.40	72.08	71.37
1	77.78	75.54	73.39	72.07	71.36
2	77.77	75.53	73.38	72.06	71.36
4	77.77	75.52	73.37	72.06	71.35
6	77.76	75.51	73.36	72.05	71.35
10	77.76	75.50	73.35	72.05	71.34
20	77.76	75.50	73.35	72.04	71.34
Hydraulic conductivity (m/day)	45.90	44.06	31.06	39.85	35.97

The second thing to do in this verification problem is to use the stochastic inverse analysis program. The initial conditions, boundary conditions, storage coefficients, the amount of discharge, and the "measured" hydraulic heads, presented in Table 5.5, are used as input in the calculations using Program 1. The steps followed in the stochastic inverse analysis are described in Section 3.5. Using the hydraulic heads given in Table 5.5, an inverse analysis provides a logarithm of hydraulic conductivity value for each zone of the aquifer. The arithmetic values of hydraulic conductivities are presented in Table 5.6.

Table 5.6 Hydraulic conductivity in each zone resulting from the inverse analysis used for the verification of the stochastic analysis program – Case 1

Zone Number	K (m/d)
1	32.56
2	32.79
3	31.44
4	31.63
5	32.04

These hydraulic conductivity values are the ones that make the total least square error between the calculated and observed hydraulic head values in all observation wells at all observation times minimum. The expected hydraulic heads everywhere in the aquifer at all times are also obtained during the inverse solution. The logarithms of hydraulic conductivity values obtained from the inverse analysis are then used to calculate the adjoint states everywhere in the study domain at all times. Both the resulting expected hydraulic heads and adjoint states at all times in all nodes are then used to calculate the Jacobians. The Jacobians, together with the logarithm of hydraulic conductivity, and hydraulic head observation values, are utilized as input in Program 2 to calculate all the covariance and cross-covariance values needed in the MLE analysis (see Section 3.3 and Appendix E). The observed hydraulic conductivity values, shown in the last row of Table 5.5, used in this calculation were determined directly from Figure 5.5 at nodes where observation wells are located. Using these observed values as input in the MLE analysis, the statistical parameters that appear in Eqs. (3.1) and (3.2) are obtained. The estimated results are μ_Y = 3.5; σ_Y^2 = 0.19; and l_Y = 97 m. These statistical parameters and the observed data are subsequently used to estimate the hydraulic conductivity distribution in the entire domain using cokriging method (Program 3). The resulting hydraulic conductivity distribution in the entire aquifer is presented in Figure 5.6 and the resulting variance distribution obtained from the cokriging estimation is shown in Figure 5.7. This step completes the stochastic inverse analysis.

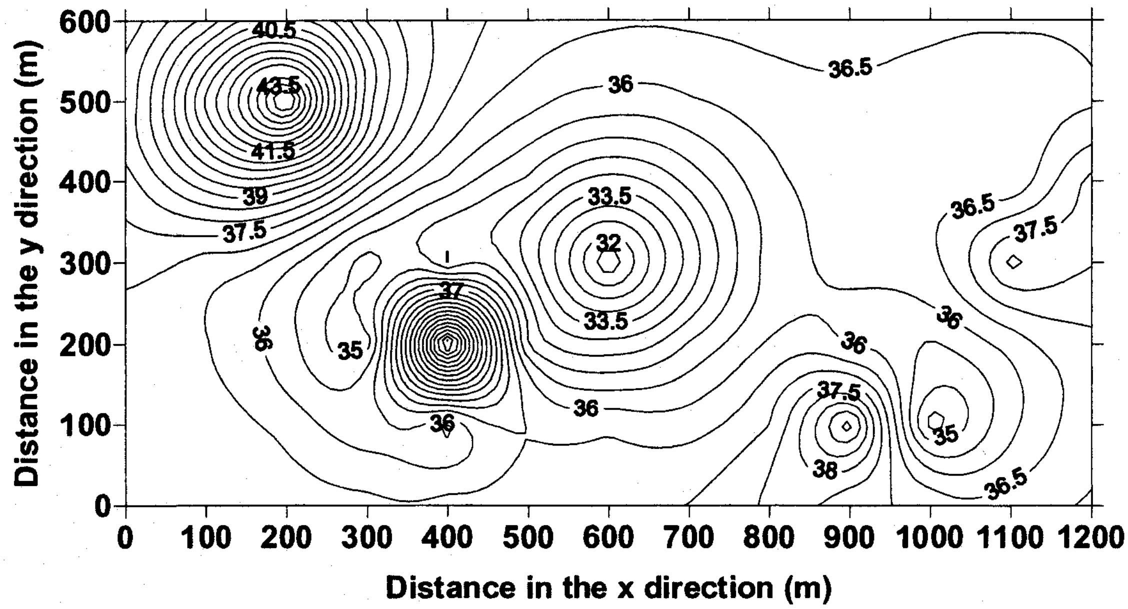


Figure 5.6 The estimate of hydraulic conductivity distribution (m/d). This figure is used in the verification of the stochastic analysis program – Case 1

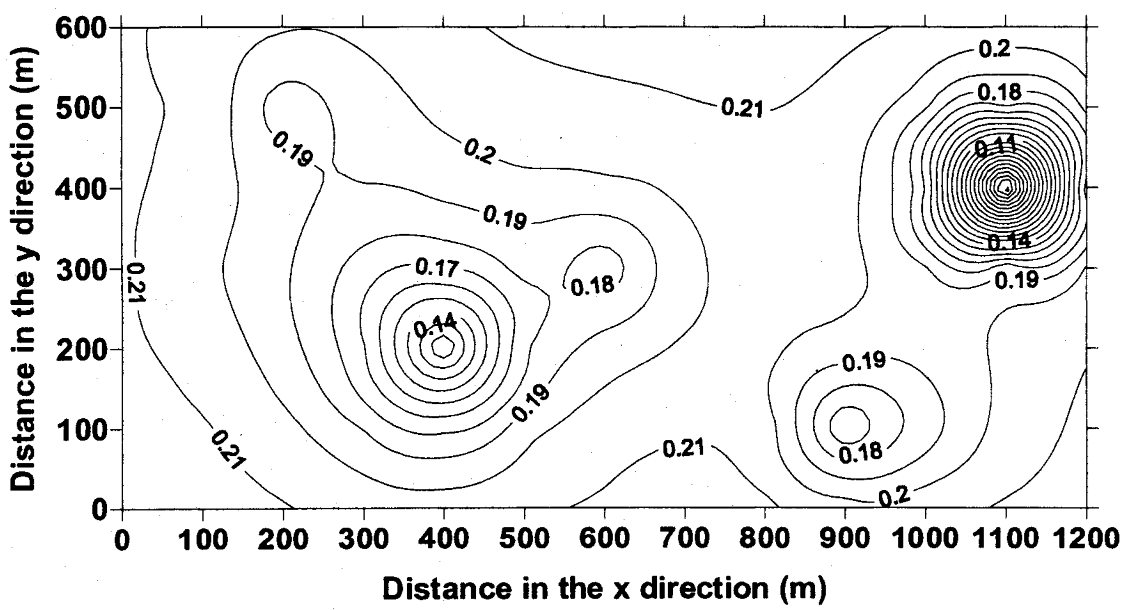


Figure 5.7 The variance distribution of the logarithm of hydraulic conductivity. This figure is used in the verification of the stochastic analysis program – Case 1

5.1.2.2 Discussion on the verification of stochastic analysis program – Case 1

The calculated values of hydraulic conductivity shown in Figure 5.6 can now be compared with the "true" values given in Figure 5.5. From the two figures it can be seen that, at some parts of the domain mostly at locations around the observation wells, the patterns of hydraulic conductivity distributions resemble. However, the values of hydraulic conductivity at some nodes do not compare well. Nevertheless, the value of L2-norm, as explained in Section 3.4, is 0.18, which can be considered as an acceptable value.

Following Flavelle (1992), regression analysis using ordinary least squares (OLS) method is used to examine the relationship between the "true" and the estimated values of hydraulic conductivity at all nodal points. The method is explained, for example, by Montgomery and Peck (1982). The plot of the regression line between the "true" and estimated values of hydraulic conductivity at all nodes is shown in Figure 5.8. From this figure it can be seen that there is a weak correlation between the "true" and estimated values. Moreover, the strength of correlation can be examined using the test statistic F_0 ($F_{1,n-1}$ distribution). The null hypothesis H_0:$\beta_1 = 0$ (where β_1 is the slope of the regression line) is rejected since the value of $F_0 > F_{0.05,1,89}$ ($F_0 = 5.87$ and $F_{0.05,1,89} = 3.96$). The P-value for the intercept and slope are 5.78^{-44} and 0.017, respectively. It can be said that the intercept and slope are slightly different from zero and it means that the "true" and estimated values of hydraulic conductivity are weakly correlated. The "true" and estimated values of hydraulic conductivity do not have a one to one correlation at each node in the study domain. However, a regression analysis is most commonly performed to show correlation between observed and estimated values at observation points. Therefore, in this thesis, regression analysis is also performed between observed hydraulic conductivity values and their estimates at observation wells. The plot of the regression line between the observed and estimated values of hydraulic conductivity is also shown in Figure 5.8. From this figure it can be seen that there is a correlation between the observed and estimated values. Moreover, the strength of correlation can be examined using the test statistic F_0 ($F_{1,n-2}$ distribution). The null hypothesis H_0:$\beta_1 = 0$ is rejected since the value of $F_0 > F_{0.05,1,3}$ ($F_0 = 89.5$ and $F_{0.05,1,3} = 10.13$). The P-value for the intercept and slope are

0.18 and 0.003, respectively. It can be said that the intercept is almost zero and slope is significantly different from zero. This means that the observed and estimated values of hydraulic conductivity are strongly correlated.

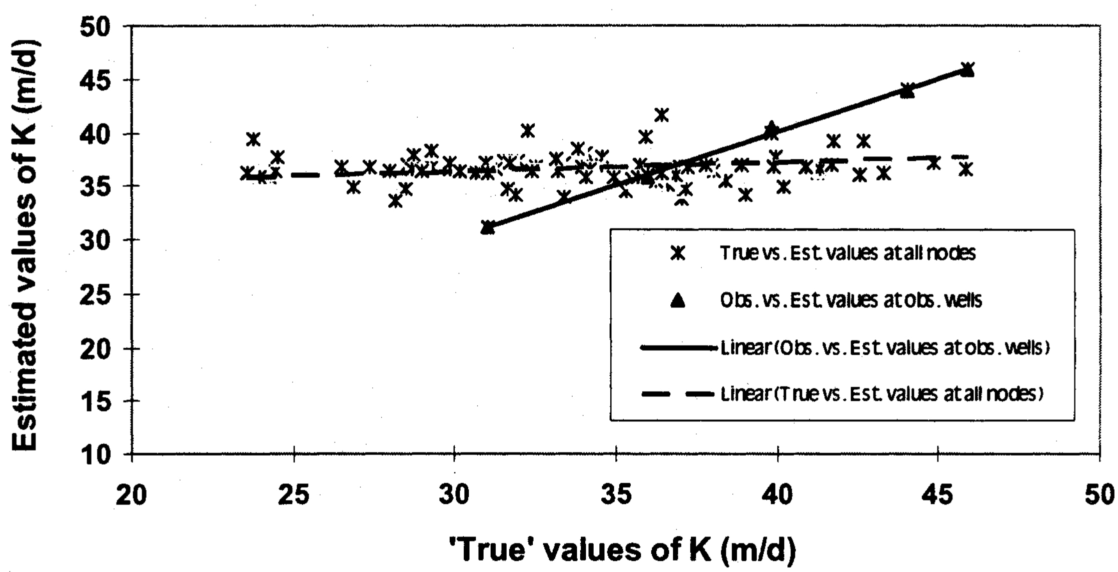


Figure 5.8 The correlation between the "true" and estimated values of hydraulic conductivity at all nodes and the correlation between the observed and estimated values of hydraulic conductivity at observation wells. This figure is used in the verification of the stochastic analysis program – Case 1

5.1.2.3 Verification of stochastic analysis program – Case 2

The second verification case makes use of a problem available in Sun and Yeh (1992). Sun and Yeh provided the "true" values of the logarithm of hydraulic conductivity in a hypothetical aquifer, which are developed using the turning bands method (Matheron, 1973; Mantoglou and Wilson, 1982). The model domain has a (240 x 560) m^2 area in plan view and is shown in Figure 5.9. Sides $\overline{AB}$ and $\overline{DE}$ are the constant head boundaries with hydraulic heads of 90 and 100 metres, respectively. Sides $\overline{BCD}$ and $\overline{EFA}$ are the "no flow" boundaries. The initial values of hydraulic heads are linearly distributed between the two constant head values at the boundaries and are presented in Figure 5.10. The distribution of 'true' hydraulic conductivity in the aquifer is given in Figure 5.11. Note that in the original figure, the logarithmic values of hydraulic conductivity are plotted.

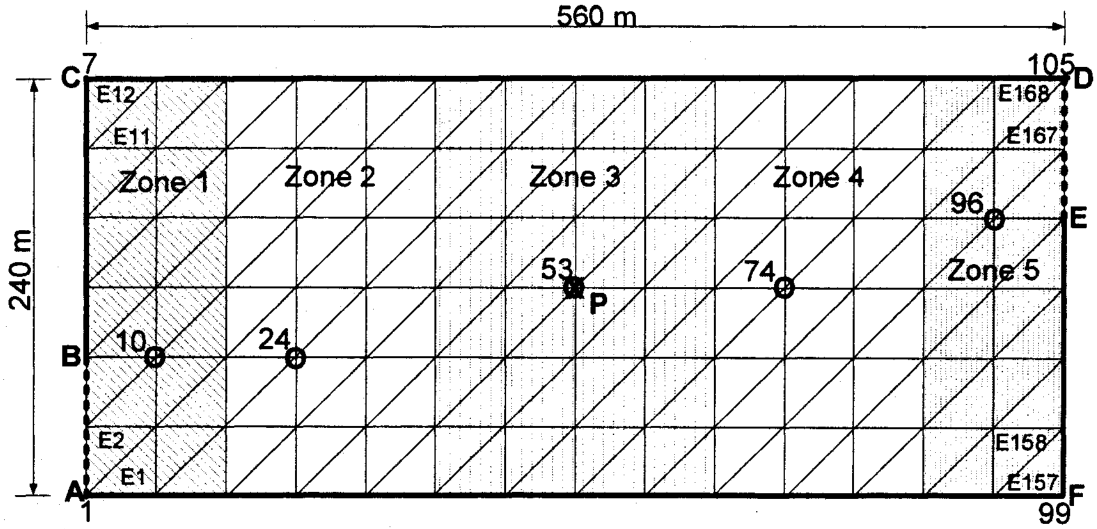


Figure 5.9 Plan view of model domain of the hypothetical problem used for the verification of the stochastic analysis program – Case 2

Legend: O = An observation well P = A pumping well
$\overline{AB}$ and $\overline{DE}$ = Constant hydraulic heads
$\overline{BCD}$ and $\overline{EFA}$ = No flow across the boundaries

The model domain is divided into 168 finite elements with 105 nodes. Five parameter zones are assumed in the domain. They are zone 1, from element 1 to 24, zone 2, from element 25 to 60, zone 3, from element 61 to 108, zone 4, from element 109 to 144, and zone 5, from element 145 to 168. The storage coefficient in all zones is assumed constant with the value of 10^{-4}. The thickness of the aquifer is also assumed constant with the value of 50 metres everywhere.

A pumping test was conducted at node 53. The observation wells for hydraulic heads and hydraulic conductivities are at nodes 10, 24, 53, 74, and 96. The pumping discharge is 4000 m^3/day. The 'observed' hydraulic head and hydraulic conductivity values are presented in Table 5.7. The observed hydraulic heads are obtained using the same method described in Case 1 (see steps 5, 6 and 7 in Section 5.1.2). The observed hydraulic conductivity values are read directly from Figure 5.11 at the nodes where observation wells are located. The calculated values of hydraulic conductivity obtained from the inverse solution analysis for zones 1 to 5 are 17.58, 16.76, 19.61, 17.72, and 23.55 m/day, respectively.

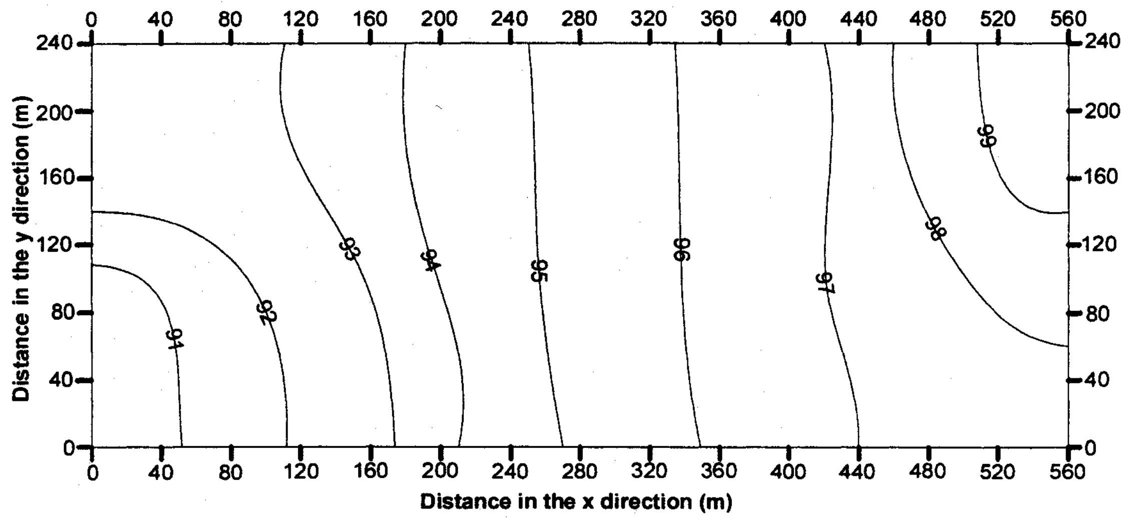


Figure 5.10 The initial values of hydraulic head in the aquifer (m). This figure is used in the verification of the stochastic analysis program – Case 2 (From Sun and Yeh, 1992).

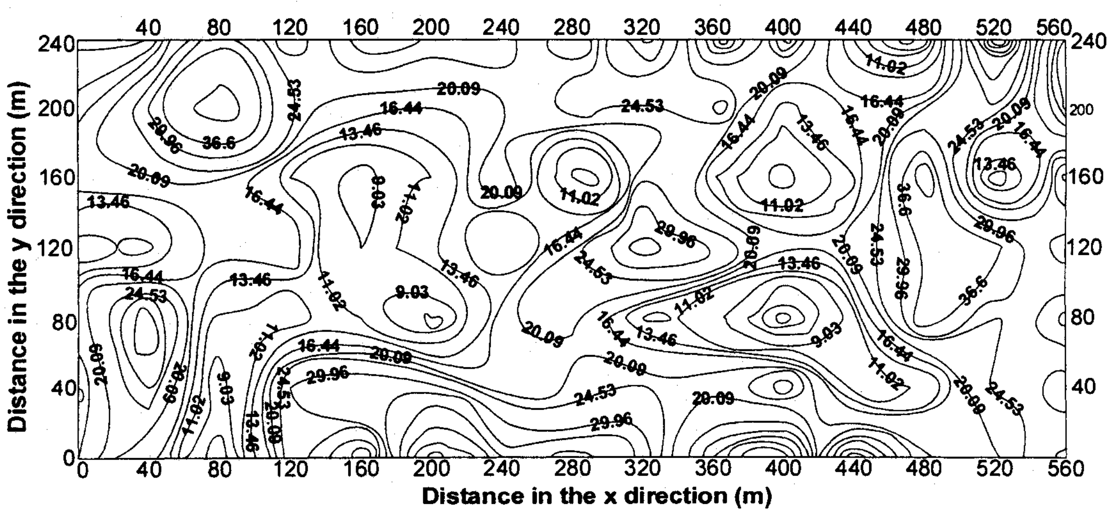


Figure 5.11 The distribution of 'true' values of hydraulic conductivity (m/d). This figure is used in the verification of the stochastic analysis program – Case 2. (This figure is a reproduction of Fig. 7.4.2 in Sun and Yeh, 1992).

Table 5.7 'Observed' values of hydraulic heads and hydraulic conductivities used for the verification of the stochastic analysis program – Case 2

Time (day)	Hydraulic heads (m) at five observation wells: 1	2	3	4	5	Node	K (m/d)
0.05	90.57	91.28	91.31	95.04	98.46	10	45.00
0.1	90.56	91.25	91.27	95.01	98.45	24	10.28
0.5	90.55	91.23	91.24	94.99	98.44	53	23.69
1	90.54	91.22	91.23	94.97	98.44	74	18.47
4	90.53	91.19	91.18	94.94	98.42	96	10.50
6	90.52	91.18	91.17	94.93	98.42		
10	90.52	91.17	91.15	94.91	98.42		
20	90.51	91.16	91.14	94.90	98.41		
30	90.51	91.15	91.13	94.90	98.41		
50	90.51	91.15	91.13	94.90	98.41		

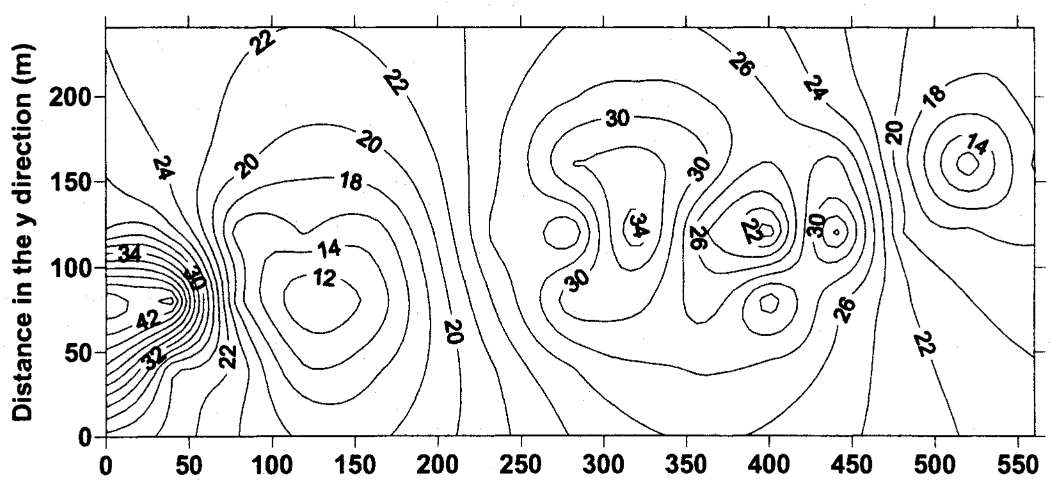


Figure 5.12 The estimate of hydraulic conductivity distribution (m/d). This figure is used in the verification of the stochastic analysis program – Case 2.

The information presented so far in this section is utilized to estimate the distribution of hydraulic conductivity in the aquifer using the stochastic inverse analysis program. The resulting statistical parameters obtained from the MLE are $\mu_Y = 2.94$; $\sigma_Y^2 = 0.04$; and $l_Y = 200$ m. The hydraulic conductivity distribution in the aquifer is estimated and the results are shown in Figure 5.12. The variance distribution is provided in Figure 5.13.

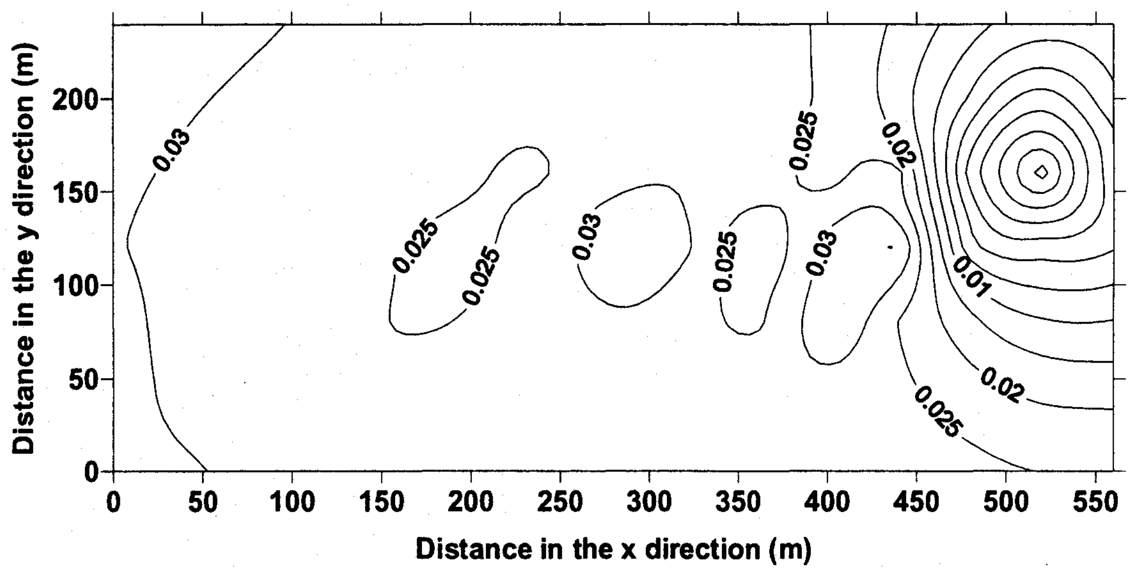


Figure 5.13 The variance distribution of the logarithm of hydraulic conductivity. This figure is used in the verification of the stochastic analysis program – Case 2.

5.1.2.4 Discussion on the verification of stochastic analysis program - Case 2

At some parts of the aquifer, mostly near the observation wells, the estimated hydraulic conductivity distribution is similar to the distribution of the "true" hydraulic heads although they are not identical. The value of L2-norm between these two distributions is about 0.57. This value shows an agreement between the two distributions of hydraulic conductivities.

A regression analysis between the "true" and estimated values of hydraulic conductivity at all nodal points is performed. The regression line can be seen in Figure 5.14. This line shows that there is a weak correlation between the "true" and estimated values of hydraulic conductivity. The value of F_0 for the Case 2 is 1.79 while the value of $F_{0.05,1,103} = 3.94$. The F_0 is less than $F_{0.05,1,103}$; therefore, the slope is considered as zero. The P-value for the intercept and parameter are 9.25x 10^{-5} and 0.18 respectively. These values show that the intercept is significantly different than zero; however, the slope is almost zero. Moreover, the P-value is big. Therefore, it can be said that there is no significant correlation between the "true" and estimated values of hydraulic conductivity. Similar to the Case 1 of verification, in Case 2 there is no one to one correlation between the "true" and estimated values of hydraulic conductivity at each node in the study domain. However, regression analysis between the observed and estimated values of hydraulic conductivity at observation wells, presented in Fig. 5.14, shows that there is correlation between the observed and estimated values of hydraulic conductivity. The value of F_0 for the Case 2 is 2949.85 while the value of $F_{0.05,1,3}$ = 10.13. The P-value for the intercept and the parameter are 0.43 and 1.37 x 10^{-5}, respectively. These values show that the intercept is almost zero and the slope is different than zero. Therefore, it can be said that there is a correlation between the observed and estimated values of hydraulic conductivity.

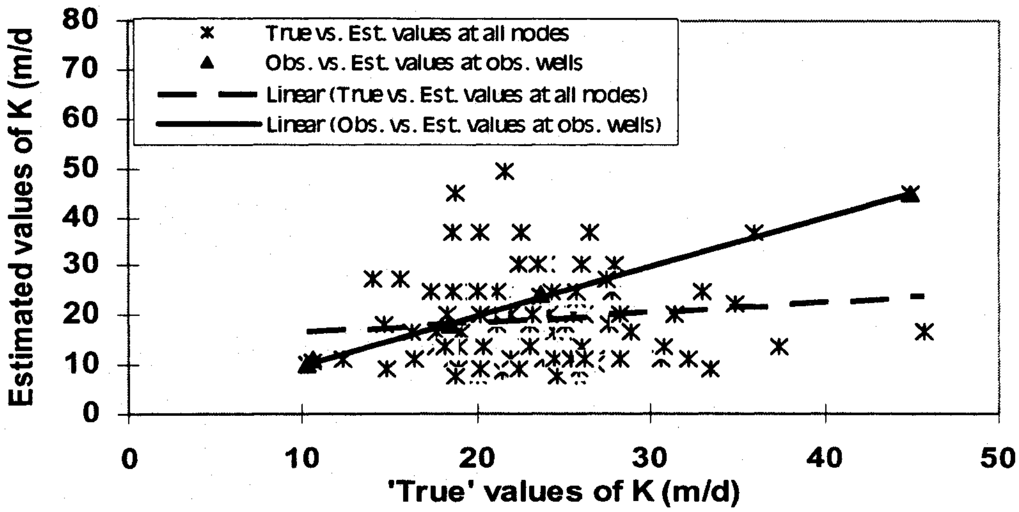


Figure 5.14 The correlation between the "true" and estimated values of hydraulic conductivity at all nodes and the correlation between the observed and estimated values of hydraulic conductivity at observation wells. This figure is used in the verification of the stochastic analysis program – Case 2

5.1.2.5 Summary of verification analyses

The results of regression analysis presented in Figs. 5.8 and 5.14 for Case 1 and Case 2 show that there is a weak correlation between the "true" and estimated values of hydraulic conductivity in the aquifer. There is no one to one correlation between the "true" and estimated values of hydraulic conductivity. Nevertheless, the correlation between observed and estimated values of hydraulic conductivity at observation wells exists. At some parts of the aquifer, mostly at the locations around the observation wells, the patterns of the estimated hydraulic conductivity distributions in both cases are similar to those of the distributions of "true" values. However, at some points other than the observation wells in the aquifer, the estimated values of hydraulic conductivity are not identical to the 'true' values. The reason for this discrepancy can be explained as follows. In the stochastic inverse analysis, the distributions of hydraulic conductivity in the aquifer are obtained from the cokriging method. In this method, the covariance functions used in the calculations are obtained by utilizing the measured values of hydraulic conductivity and hydraulic heads at the observation wells. The hydraulic conductivities at all other points in the aquifer are obtained from the interpolation process. In the hypothetical model, however, the distribution of the "true" values of hydraulic conductivities is obtained by a procedure described in Section 5.1.2, which is different than the cokriging method. Therefore, the estimated hydraulic conductivity values at points other than the observation points can be different from the 'true' values at these points (see also the example on pages 214-219 in Kitanidis, 1997). An increase in the number of observation wells will result in a better agreement between the "true" and estimated values of hydraulic conductivities in the aquifer. Moreover, the regression analysis is usually conducted only between the observed and estimated values of parameters. The regression analysis in this thesis, which is involving all values of hydraulic conductivity in all nodal points, in which the number of observation wells is very few (5 out of 91 for Case 1 and 5 out of 105 for Case 2), produces estimated hydraulic conductivities different from the "true" values. Therefore, it makes sense if there is no strong correlation between the "true" and estimated values of hydraulic conductivity in the aquifer. Furthermore, the objective of the estimation of the "true" values of hydraulic conductivity is not to produce estimated values of hydraulic conductivity exactly the same as the "true" values of hydraulic conductivity. The estimation procedure produces estimates of the "true" values of hydraulic conductivity such that the calculated hydraulic heads are matching with the observed hydraulic heads in the aquifer system. In addition, Sun and Yeh (1992) stated that the estimated values of hydraulic conductivity obtained from both the Gaussian conditional mean and cokriging estimates cannot be the same as the "true" values of hydraulic conductivity. "The difference between them is generally caused by: (1) the error in the statistical structure of $\hat{Y}$, (2) the error in the statistical parameters of $\hat{Y}$ obtained by the MLE, and (3) the fact that $\hat{Y}$ is usually smoother than Y^*" (Sun and Yeh, 1992).

(Note: The results of the two cases of verification are presented in Appendix F in three different forms. The residuals between the "true" and estimated values of hydraulic conductivity in the study domain are plotted. In addition, four forward analyses using MODFLOW are performed in order to determine the significance of using true or estimated hydraulic conductivity values. The hydraulic heads at the observation wells and the water balance in the aquifer calculated by forward analyses using true and estimated hydraulic conductivity values are discussed.)

The plots of the estimated hydraulic conductivities in both cases suggest that these conductivity values in the aquifer might be affected by the zonation chosen in the analysis in the present study.

The adjoint states method used in the inverse analysis is an efficient method in terms of computer storage requirement and computational time as stated by Sun and Yeh (1985) and Yeh (1986). In a general minimization procedure of the performance function with respect to hydraulic conductivity, one needs to calculate the gradient of hydraulic heads with respect to each hydraulic conductivity value. For a large number of hydraulic conductivity values, a general minimization procedure will consume a lot of time and will require a large amount of computer storage space since this gradient needs to be calculated in each iteration step. In the adjoint states method, however, the calculation of gradient of hydraulic heads with respect to hydraulic conductivity is eliminated by the adjoint equation. This equation is only solved (I x J) + 1 times for which I is the number of observation wells and J is the number of observation times to obtain the adjoint state corresponding to each observation well and observation times. There is one more simulation run to calculate the expected head distribution in the aquifer. For example in the first case of verification the number of simulation run needed is about (5 x 10) + 1 = 51 runs.

5.2 Validation/Application of Stochastic Analysis Program

In civil engineering, the validity of a computer program is confirmed by making successful predictions for the actual behaviour of structures. Validation of a computer program requires a large number of comparisons between the predictions of the computer program and the measurements taken in real life problems. All programs have limitations. They are written with certain assumptions to achieve certain goals. Therefore, comparisons should be made for problems within the limitations of the program. Validation is a continuous process. A few successful predictions do not guaranty success for all other predictions. Further discussion on this subject can be found in Konikow and Bredehoef (1992) and de Marsily et al. (1992).

There are not many full-scale field data, with sufficient details, to validate a stochastic inverse finite element program. In addition, there were no plans made in the present investigation to obtain such data from full-scale problems in the field. Therefore, the stochastic inverse program is used to solve actual field problems described in detail in the literature. Because of this reason, the validation cases in this thesis can also be considered as applications of the developed program. Field observation data are taken from two different papers as described in the following sections.

5.2.1 Validation of stochastic analysis program – Case 1

The first case of validation problems is taken from the United States Geological Survey Water-Supply Paper number 2453 written by Marie and Hollett (1996). There was a pumping test conducted in the South Vekol Valley, Arizona. The South Vekol Valley basin is located about 610 m above the sea level. It is a large, flat basin with dimensions in the order of 19-20 km in each direction and a slope of about 1.9 m/km northward. A sketch of the area is shown in Figure 5.15.

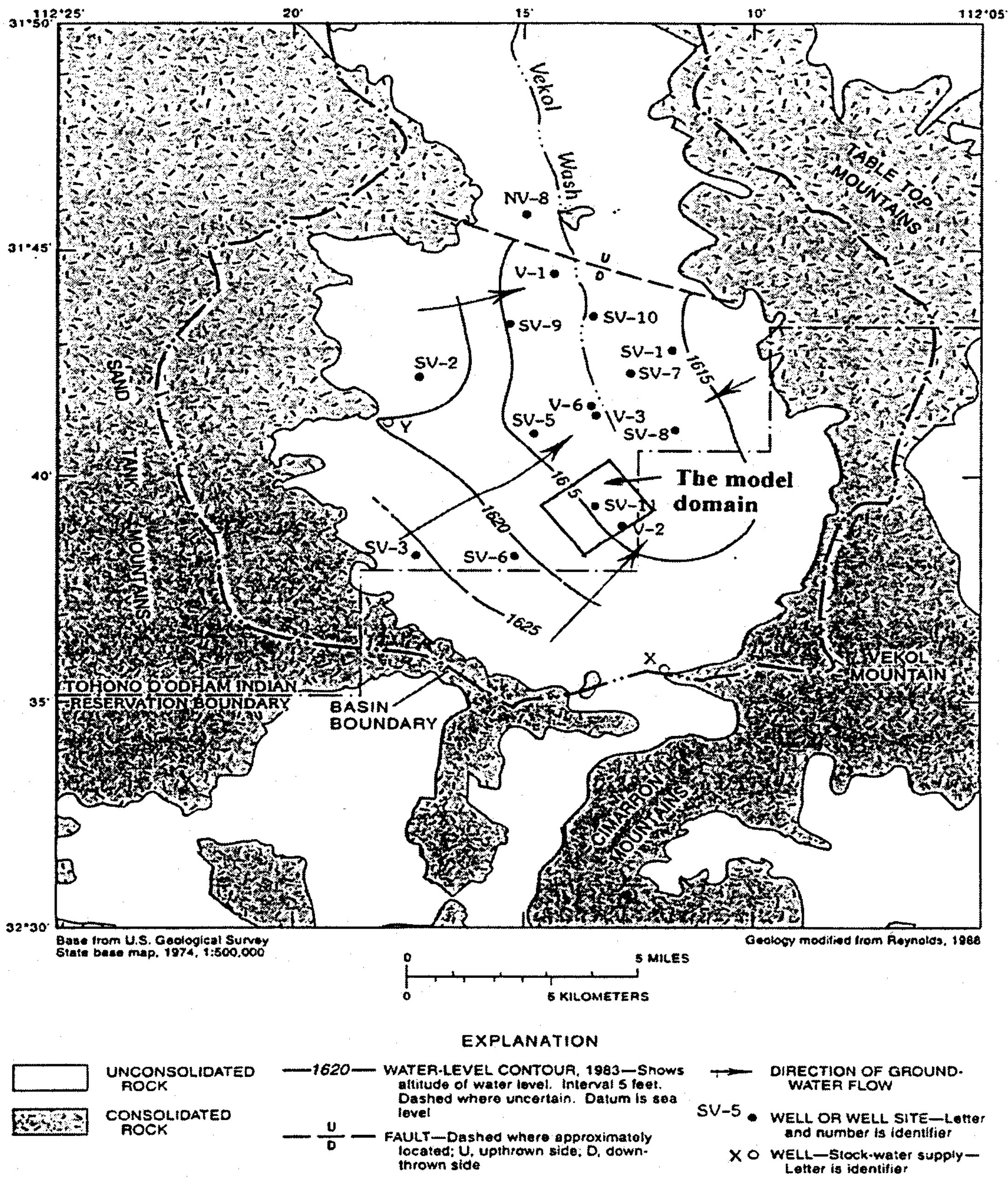


Figure 5.15 Sketch of the South Vekol Valley (from the United States Geological Survey Water-Supply Paper number 2453). This figure is used in the validation of the stochastic analysis program–Case 1.

The geological structure in the basin comprises of a sequence of layers of silt, sand and gravel. The total thickness of the layers varies from 65 m to 365 m near the perimeters. Around the centre of the aquifer, the thickness varies from about 335 m to 550 m. In most part of the basin, underlying these layers, there is a sequence of volcanic rocks with a thickness varying from 213 m to 274 m.

The aquifer is located below the silty soil layer and, as stated in the report, it is a confined aquifer. This aquifer consists of unconsolidated sand and gravel with an average thickness of about 402 metres. A small part of the aquifer at the bottom contains gravel and conglomerate. Some of this information is based on the analysis of data obtained from the boreholes SV-8 and SV-11 where the pumping tests were conducted.

In this thesis, the data from the pumping test conducted in well number SV-11 were used. The drawdown values were recorded in observation wells numbered as SV-11ob1, SV-11ob2, and V-2. These wells were located about 55 m, 155 m and 1100 m southeast of well SV-11, respectively. The farthest well that showed any response to pumping was the well V-2. There was no noticeable drawdown in wells SV-6 and SV-8. The layout for the aquifer test at well SV-11 is shown in Fig. 5.16. The pumping discharge was 24,255 m^3/day. The pumping test was conducted for 21 days. The area that is chosen for the analysis is shown in Fig. 5.15. The finite element mesh used in the analysis, boundary conditions, and initial heads are shown in Figures 5.17and 5.18. The pumping test data is presented in Figure 5.19. From the analysis of the pumping test in this area, the value of the storage coefficient in the aquifer was found to be about 0.0003. The hydraulic conductivity values varied approximately between 2.0 m/day and 5.7 m/d.

The model domain is divided into 176 elements with 108 nodes. The pumping well SV-11 is at node 59 that is located in the middle of the domain. The observation wells, which are labeled as SV-11ob1, SV-11ob2, and V-2, are located at nodes 14, 41, and 50, respectively. Constant head boundary conditions are assumed for sides labeled as $\overline{AFE}$

and $\overline{BCD}$ with the constant head similar to the initial heads at those nodes; i.e., 491.0 and 493.0 m, respectively. At sides $\overline{AB}$ and $\overline{DE}$, there is no flow across these boundaries.

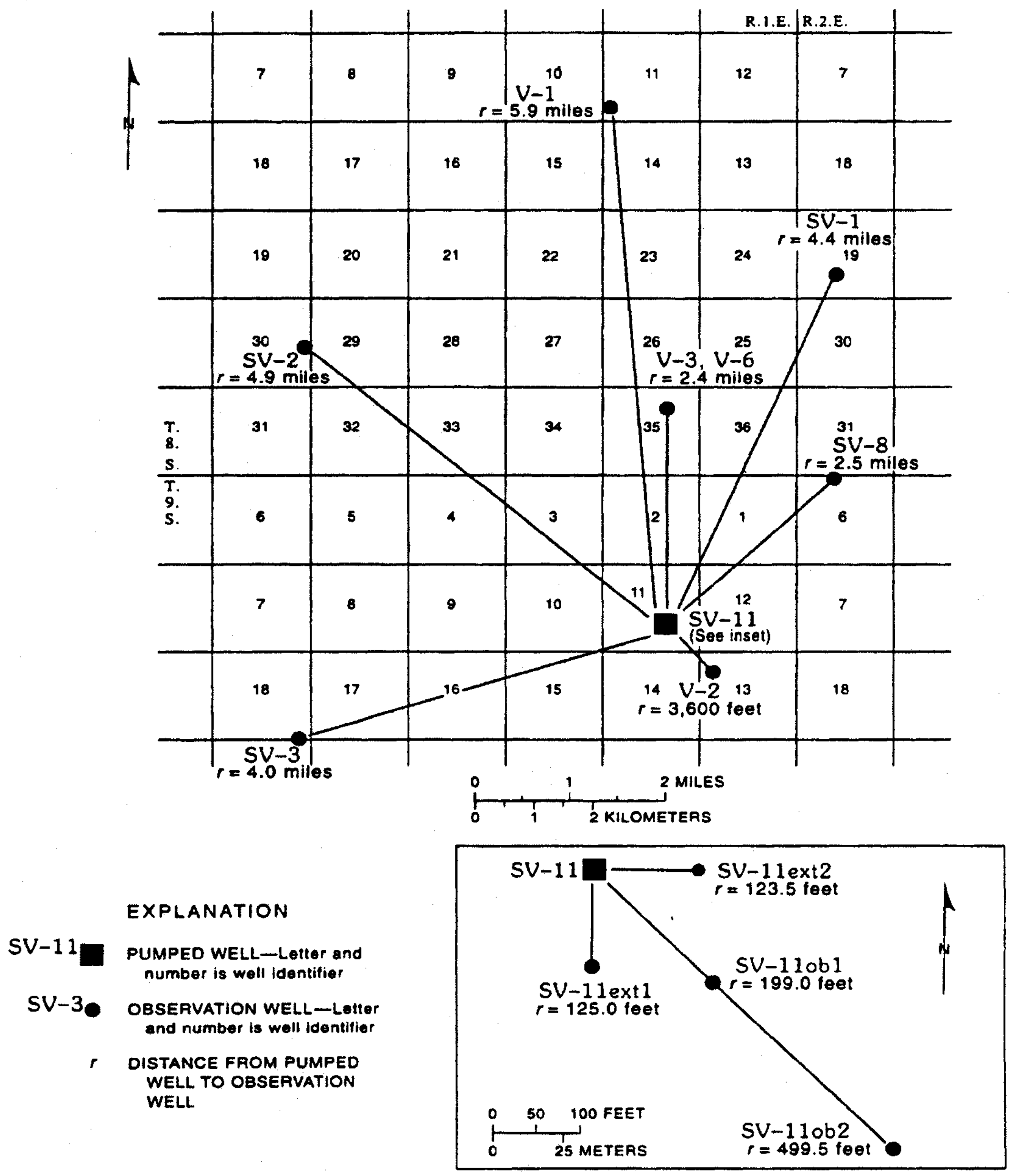


Figure 5.16 Layout for the aquifer test at well SV-11(from the United States Geological Survey Water-Supply Paper number 2453). This figure is used in the validation of the stochastic analysis program–Case 1.

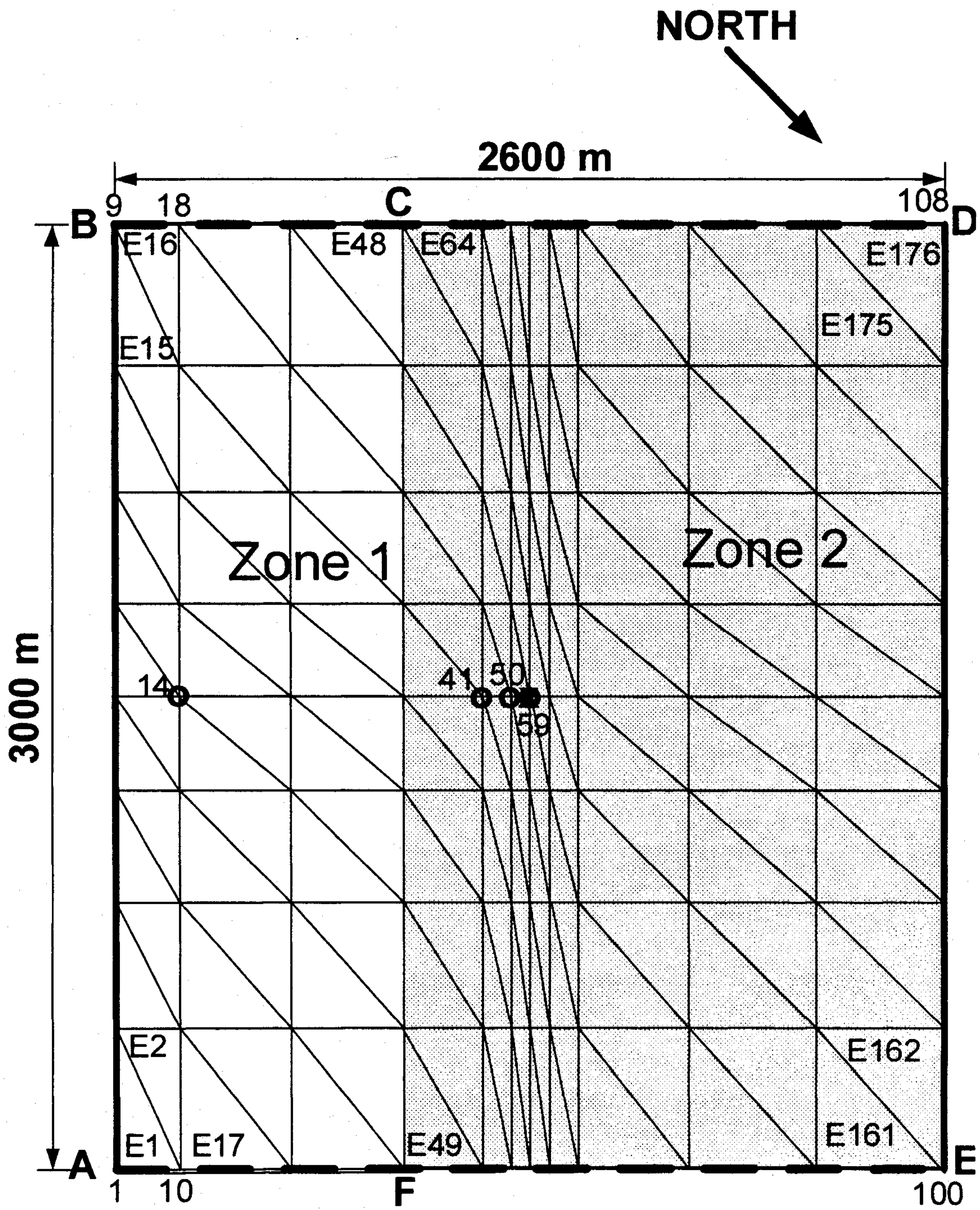


Figure 5.17 Plan view of the area of the field problem used for the validation of the stochastic analysis program–Case 1

1, 2,…,104 = Node numbers X = A pumping well

E1, E2,…,E168 = Element numbers O = An observation well

Sides $\overline{BCD}$ and $\overline{FGH}$ = Constant head boundary conditions

Sides $\overline{HAB}$ and $\overline{DEF}$ = No flow across the boundaries

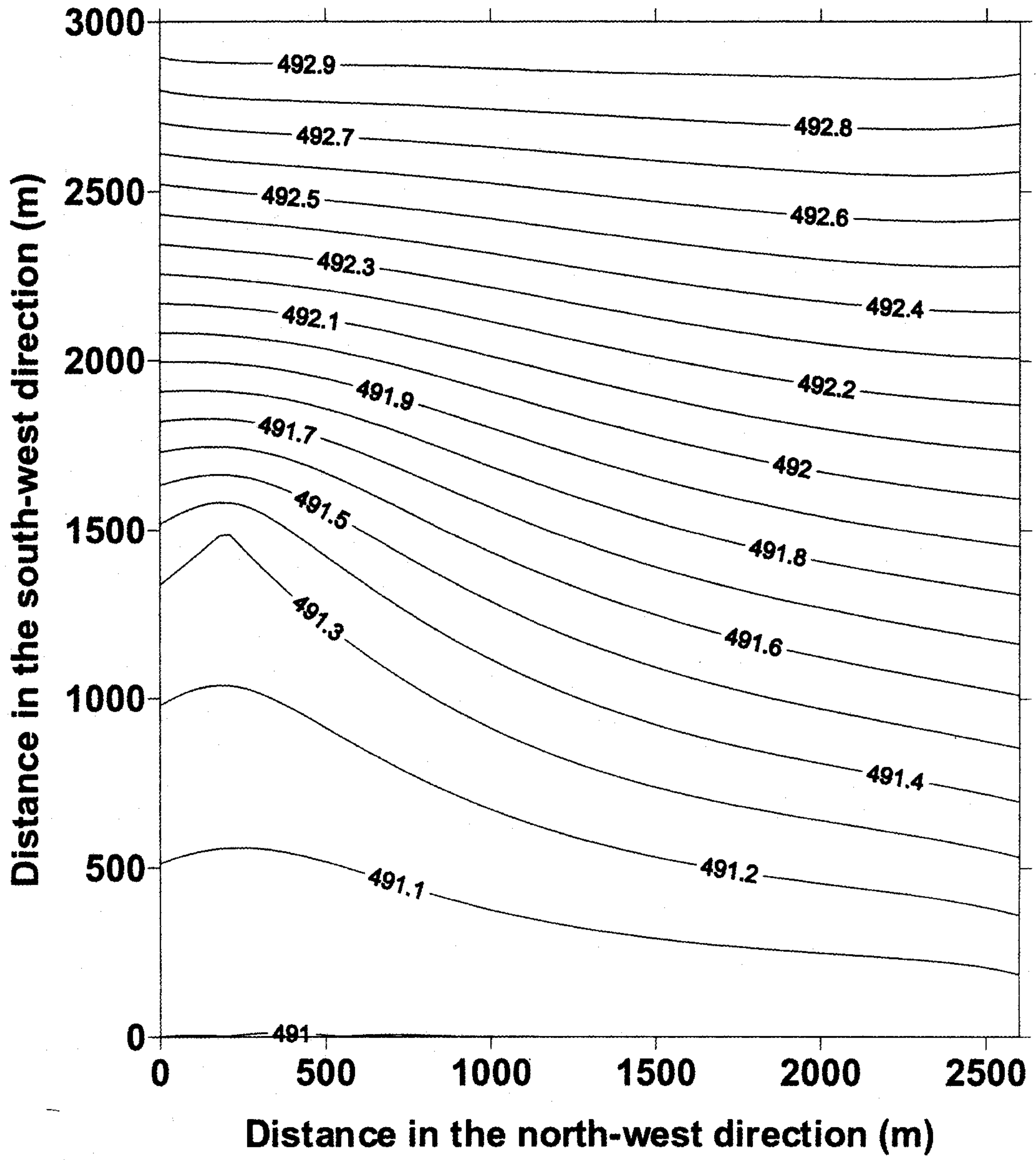
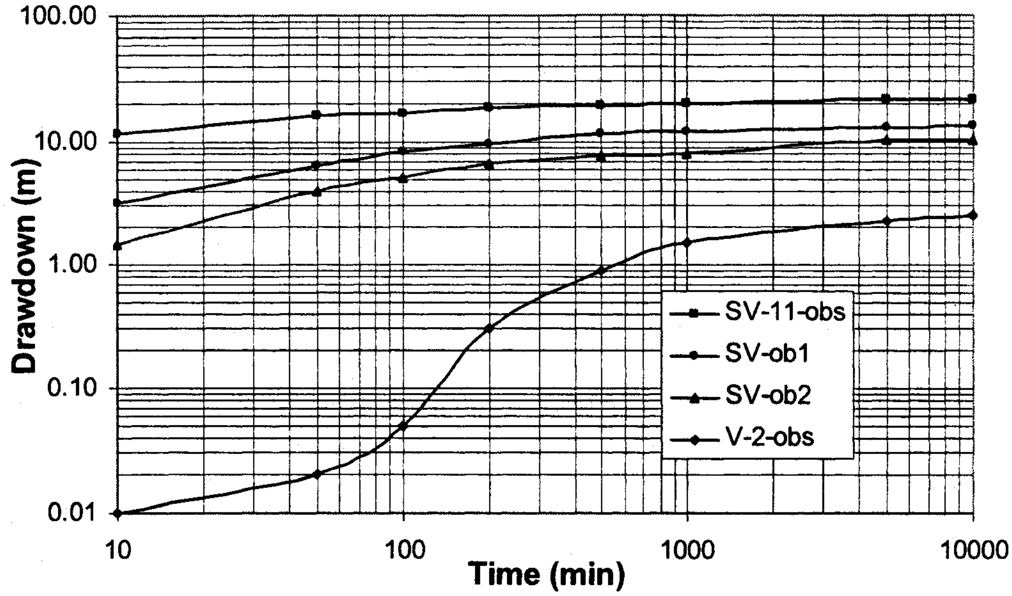


Figure 5.18 The initial head distribution (m). This figure is used in the validation of the stochastic analysis program--Case 1.

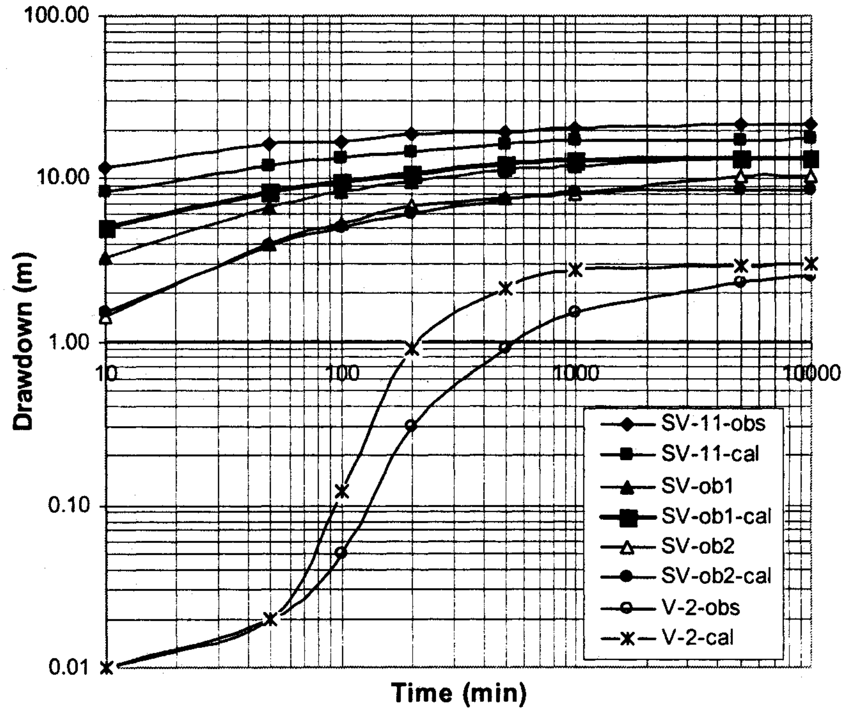


Note: obs = observed drawdown

Figure 5.19 Drawdown (m) in wells. This figure is used in the validation of the stochastic analysis program–Case 1.

5.2.1.1 Results and discussion of the validation problem - Case 1

The original drawdown data provided in the Geological Survey Water Supply paper could not be matched closely in the inverse analysis. The reason for this is the lack of detailed information related to the aquifer thickness, the boundary conditions, and the storage coefficients. Moreover, it is mentioned in the original report that the aquifer changed from a confined to an unconfined aquifer when the pumping was conducted for a long time period (21 days). In addition, the drawdown produced by the groundwater equation is usually smoother than the observed one because the measurement error usually cannot be avoided completely. The measurements related to the characteristics of the aquifer are available only at a few points. Hydraulic conductivity was measured at the pumping well SV-11 and at the observation wells SV11-ob1, SV-ob2 and V-2. Their values are about 2.07 m/day, 2.1 m/day, 2.38 m/day, and 5.61 m/day, respectively. The values of hydraulic conductivity and storage coefficient obtained from the analysis of the pumping test were the average of the whole region under consideration. Therefore, based on the available data, the locations of different zones in the aquifer are chosen. In these analyses, the aquifer is divided into two parameter zones. The choice of the location and number of zones is based on the agreement of the observed drawdown with the one used in the model. Zone 1 contains elements from 1 to 64, and zone 2 contains elements from 65 to 176. Hydraulic conductivity values for zones 1 and 2 are 4.48 m/day and 1.57 m/day, respectively. The drawdown data used for the inverse analysis in this thesis is then developed using a forward solution analysis. The drawdown resulting from the forward analysis is the best match to the original drawdown in the Geological Survey Water Supply paper.



Note: obs = observed drawdown; cal= calculated drawdown

Figure 5.20 Comparison between the original data and the data used in the model for the purpose of validation of the stochastic analysis program–Case 1

The drawdown in all wells used in the model is compared to the original data and presented in Figure 5.20. Using the developed data, the hydraulic conductivity distribution in the region is estimated. The statistical parameters obtained from the MLE method are μ_Y = 1.51; σ_Y^2 = 0.07; and l_Y = 190 m. The resulting hydraulic conductivity distribution can be seen in Figure 5.21. The distribution of the variance of hydraulic conductivity is presented in Figure 5.22.

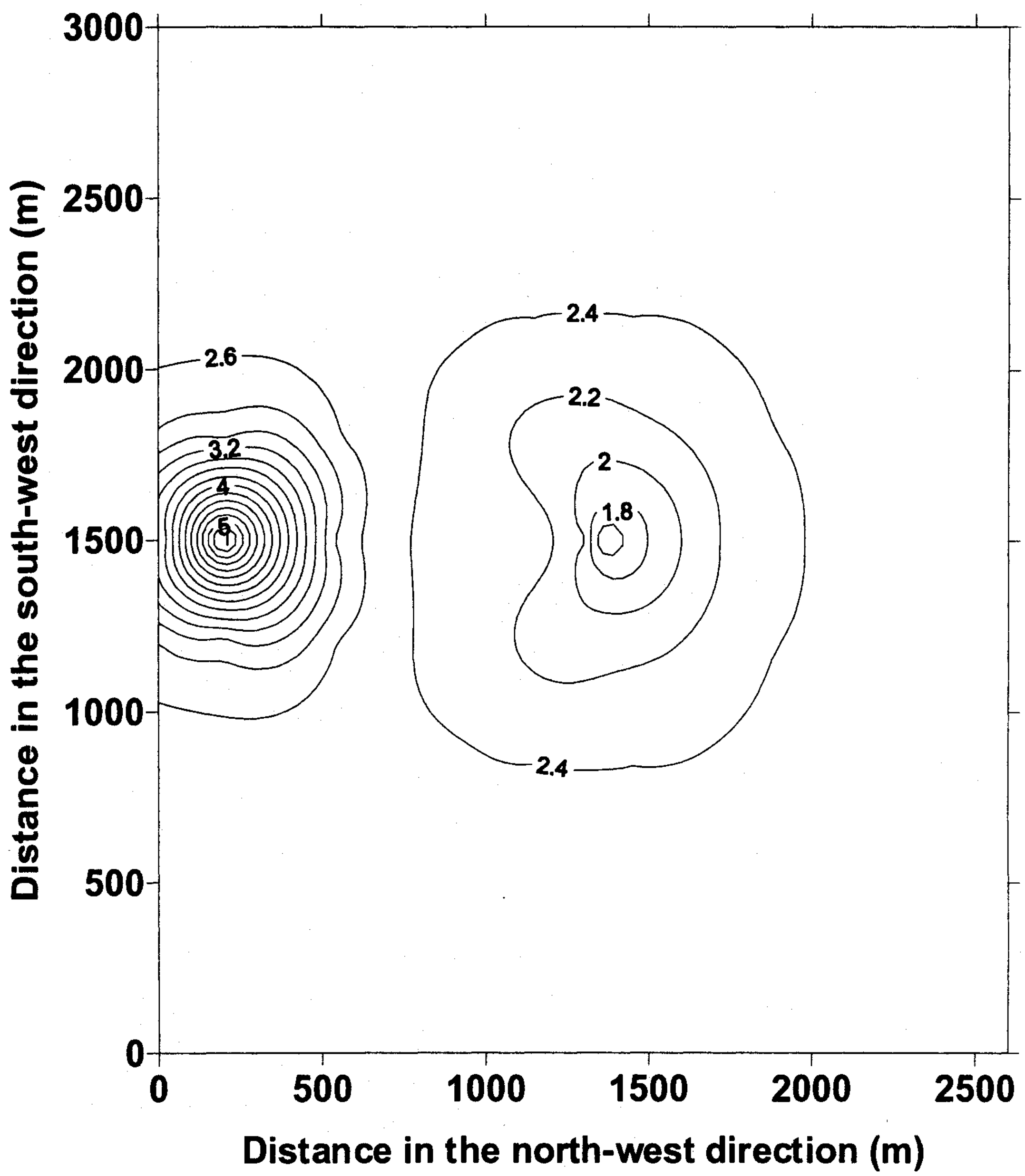


Figure 5.21 The estimated hydraulic conductivity distribution of the real field problem (m/day). This figure is used in the validation of the stochastic analysis program–Case 1.

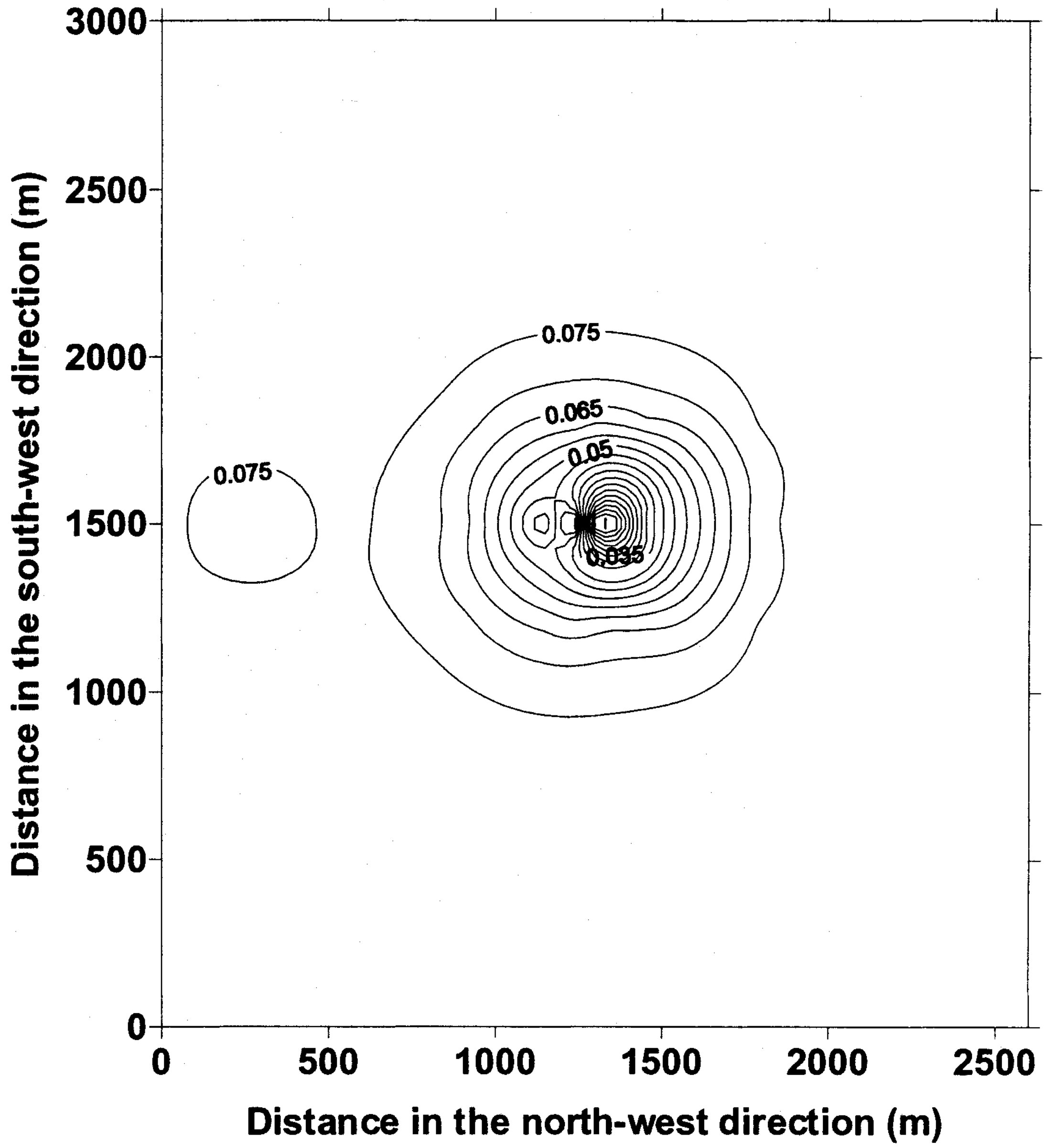
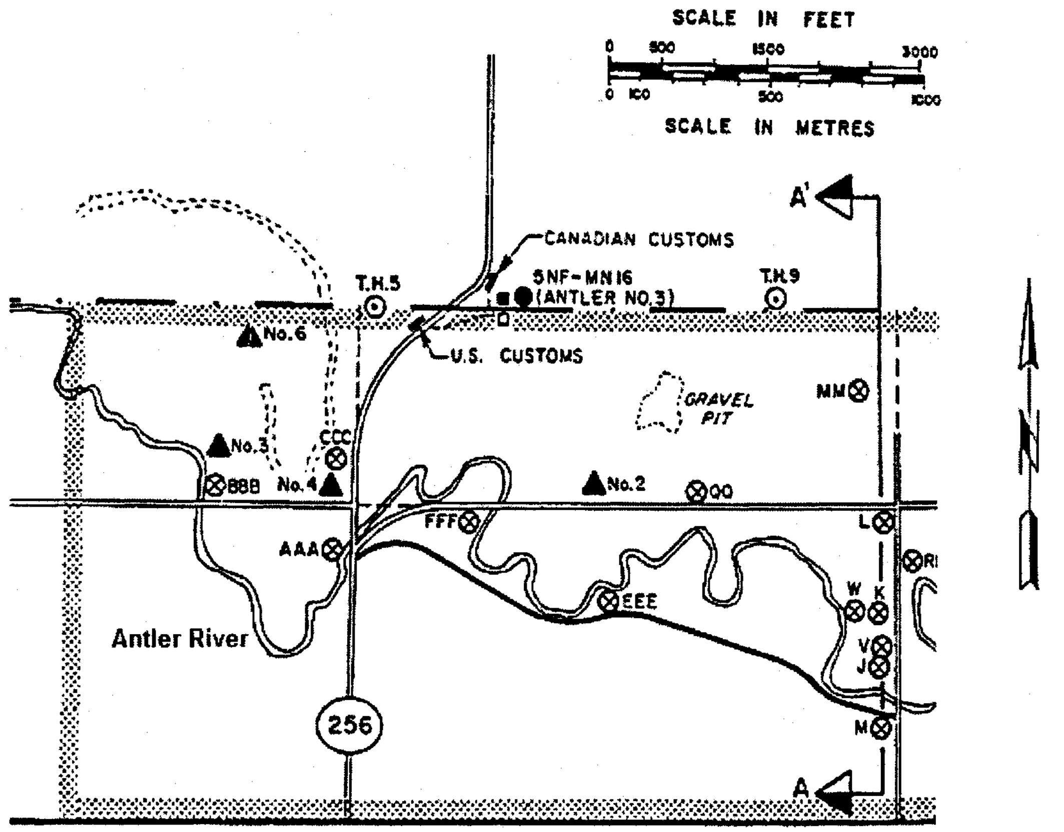


Figure 5.22 The variance distribution of the logarithm of hydraulic conductivity. This figure is used in the validation the of stochastic analysis program–Case 1

The average values of hydraulic conductivities are about 2.6 m/day and 2.3 m/day for zone 1 and zone 2, respectively. The maximum and minimum values of hydraulic conductivity in zone 1 are about 5.6 m/day and 2.3 m/day and in zone 2 are about 2.5 m/day and 1.4 m/day. Most of these values are within the range of the hydraulic conductivities provided in the original paper although the minimum value of the estimated value is less than the minimum value given in the paper.

5.2.2 Validation of stochastic analysis program – Case 2

A published report about the Antler River Aquifer Investigation (Rutulis, 1977) is used for the second case study in this thesis. The aquifer is located in the province of Manitoba. A plan view of the aquifer around the pumping wells and its boundaries are shown in Figures 5.23 and 5.24, respectively. Labels AS and AR provided in these figures indicate the names of the investigators; i.e. All Seasons Water Users Association Inc. and Antler River Aquifer Investigation.



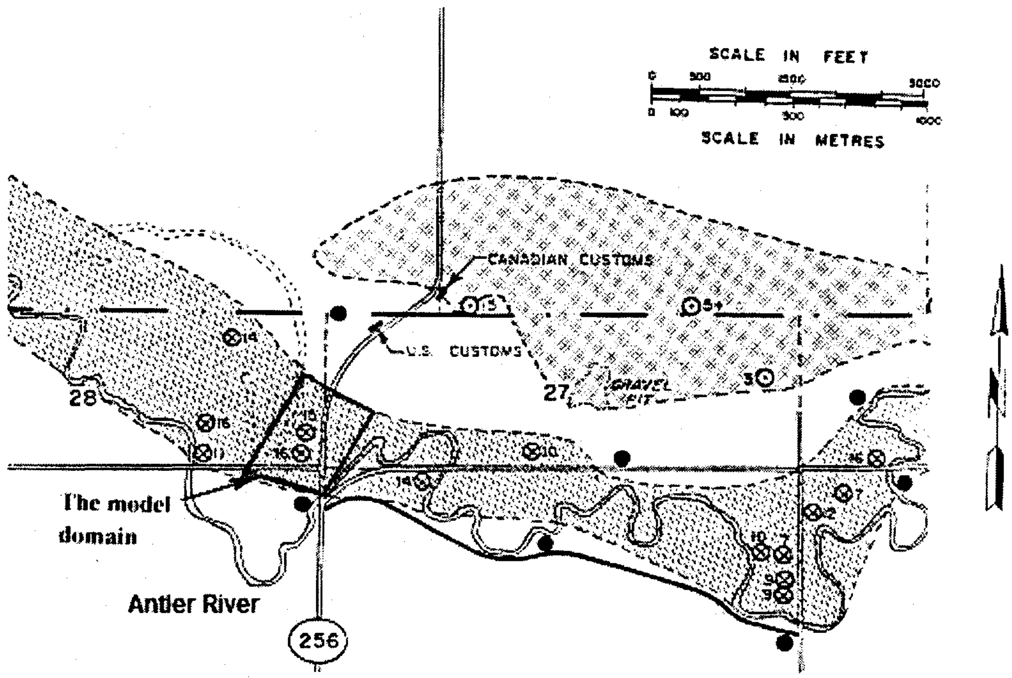
▲ = a pumping well as well as a test hole (AS), (⊗ = a test hole (AS)

⊙ = a test hole (AR), • = an observation well (AR)

Figure 5.23 Plan view of the aquifer around production wells (from Rutulis, 1977). This figure is used in the validation of the stochastic analysis program–Case 2.

The aquifer is confined between a layer of silt and clay at the top and a glacial till deposit at the bottom. The thickness of the aquifer is not constant. The most common thickness is

3 metres. The values of transmisivity of the aquifer are between 596 m2/day to 1193 m2/day. For the average thickness of 3 metres, the value of the hydraulic conductivity ranges between 198 m/day to 398 m/day. The value of the storage coefficient is between 10-3 to 10-4. A cross section of the aquifer at the location indicated in Figure 5.23 is shown in Figure 5.25.



⊗ = a test hole (AS), ⊙ = a test hole (AR), • = an observation well (AR)

Figure 5.24 The boundaries of the aquifer (from Rutulis, 1977).
This figure is used in the validation of the
stochastic analysis program–Case 2.
Note: Numbers written close to test holes indicate the thickness
of the aquifer at those locations. The unit of dimensions is in feet.

For the purpose of modeling, a small region of the aquifer around a pumping well (No. 4) is chosen. This region, $\overline{ABCDEF}$, is 300 metres long and 380 metres wide. The finite element mesh representing this region is divided into 108 elements with 70 nodes as shown in Fig. 5.26. The hydraulic head in the region is determined from the location of the piezometric surface provided in Fig. 5.25, although this cross-section was outside the model domain. The sides of the region indicated by $\overline{ABC}$ and $\overline{DEF}$ are the constant head boundaries with 461 metres head along both sides. The sides labeled as $\overline{AF}$ and $\overline{CD}$ in Fig. 5.26 do not have any flow across these boundaries. The initial heads in the aquifer are assumed to have the same value of 461 m everywhere.

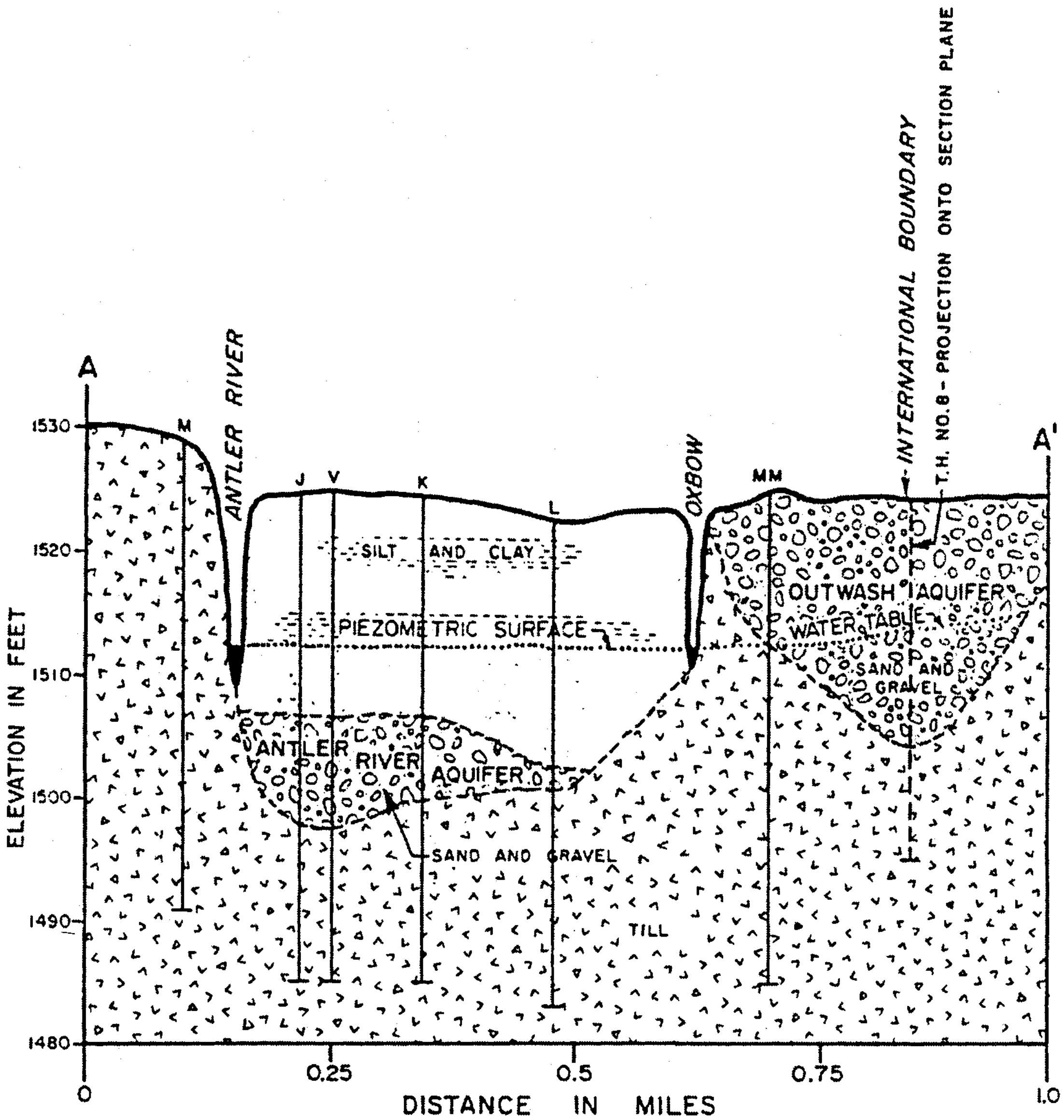


Figure 5.25 The A – A′ cross section (from Rutulis, 1977). This figure is used in the validation of the stochastic analysis program–Case 2.

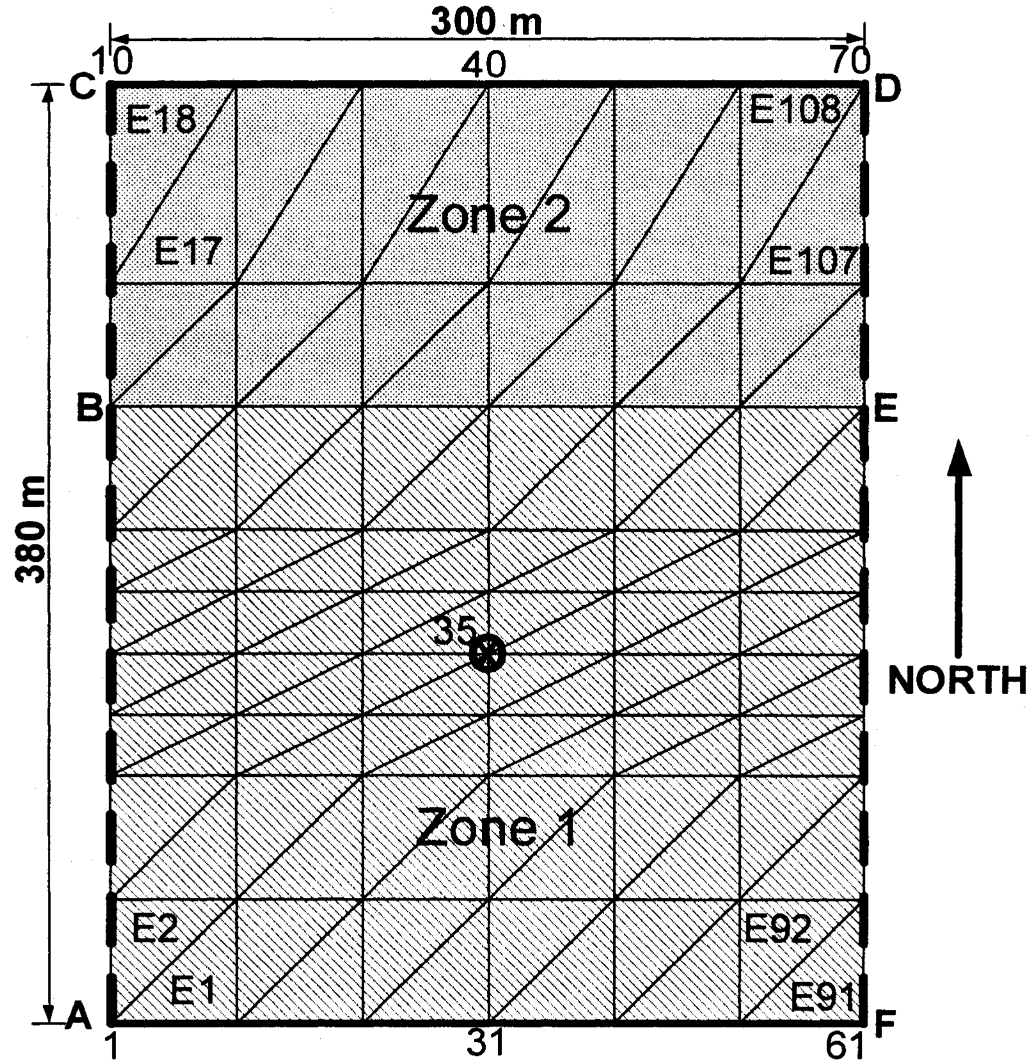


Figure 5.26 Plan view of the hypothetical area of the field problem used for the validation of the stochastic analysis program–Case 2

1, 2,…,70 = Node numbers X = A pumping well

E1, E2,…,E108 = Element numbers O = an observation well

Sides $\overline{ABC}$ and $\overline{DEF}$ = Constant head boundary conditions

Sides $\overline{AF}$ and $\overline{CD}$ = No flow across the boundaries

The finite element domain is divided into two zones. Zone 1 comprises the elements within the region labeled as ABEF. The region indicated by BCDE is chosen as Zone 2. The storage coefficient in the aquifer is assumed to be 0.0002 everywhere. The hydraulic conductivities are assigned values of 200 m/day and 395 m/day for nodes 35 and 39, respectively, based on the available information about the hydraulic conductivities in the whole aquifer. Similar to the validation Case 1, the determination of location and number of zones in this case were also based on the agreement between the measured drawdown and the one used in the model.

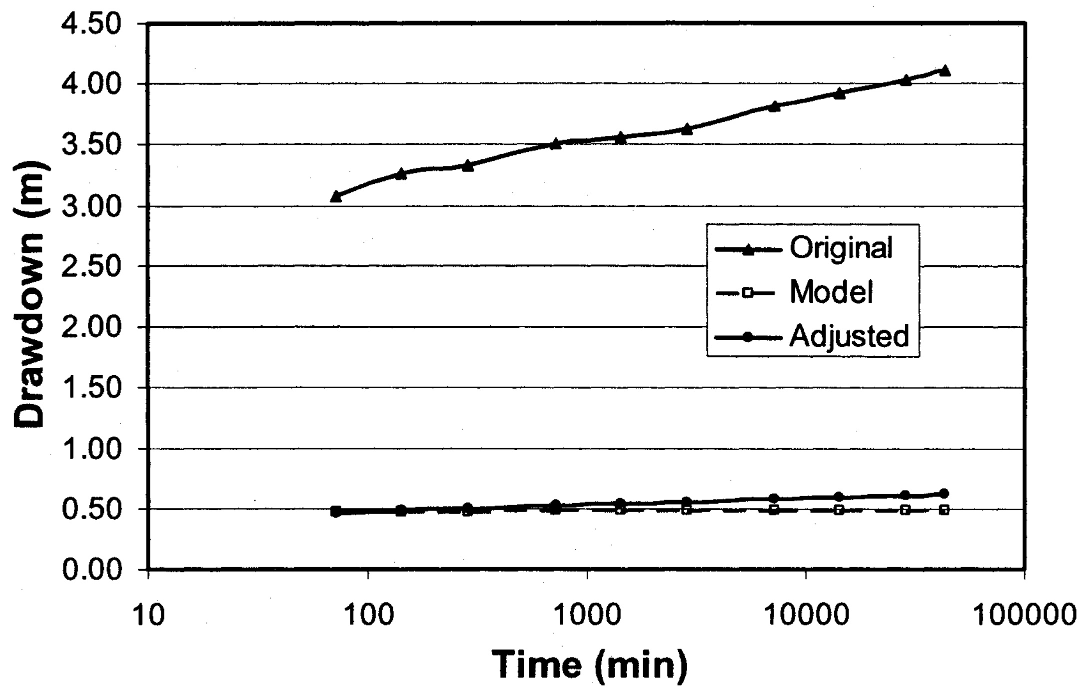


Figure 5.27 The drawdown (m) in well number 4. This figure is used in the validation of the stochastic analysis program–Case 2.

Various pumping tests were conducted at a number of different wells in the region. In this investigation, the data collected at the pumping well No. 4 is used in the analysis (see Figure 5.23). The discharge at this well was about 350 m^3/day. The resulting drawdown at the pumping well was about 2.5 metres after (about 1 minute) the pumping was initiated, and 3.5 metres at the end of pumping period (1100 minutes). However, it is noted in the report that a large part of the drawdown in the pumping well was due to the well loss. It was concluded in the report that the real drawdown at the end of the pumping test was less than 61 cm. Similarly, the drawdown data to be used in the present calculations required some adjustments to the drawdown values given in the report so that the effect of the well loss could be accounted for. The adjusted drawdown is chosen to be about 15 % of the unadjusted, measured value of drawdown. As a result, the present analysis uses a value of 61 cm for drawdown at the end of the pumping test. In the finite element model, the pumping well is located at node 35. Using the information of hydraulic conductivity values in the aquifer, a forward analysis was conducted. A very good match is obtained between the calculated drawdown and the measured, adjusted drawdown data in the well as shown in Figure 5.27. This drawdown was obtained when the values of hydraulic conductivity in zone 1 and 2 were 123 m/day and 391 m/day, respectively.

5.2.2.1 Results and discussion of the validation problem - Case 2

The drawdown data obtained from the forward solution analysis and the measured values of hydraulic conductivity are used to estimate the hydraulic conductivity distribution in the aquifer. The statistical parameters obtained from the MLE method are $\mu_Y = 5.8$; $\sigma_Y^2 = 0.08$; and $l_Y = 66$ m. The resulting hydraulic conductivity distribution and its variance are presented in Figure 5.28 and 5.29, respectively. The average values of hydraulic conductivity in zone 1 and 2 are about 206 m/day and 243 m/day, respectively. The minimum and maximum values of the hydraulic conductivity in zone 1 are about 169 m/day and 237 m/day while in zone 2 are about 221 m/day and 395 m/day, respectively. These values are within the range of the observed values given in the original report.

The intension of this section was to validate the program; however, available field data did not have sufficient amount detailed information for validation. Therefore, the problems analyzed for validation purpose can be considered only applications of the method.

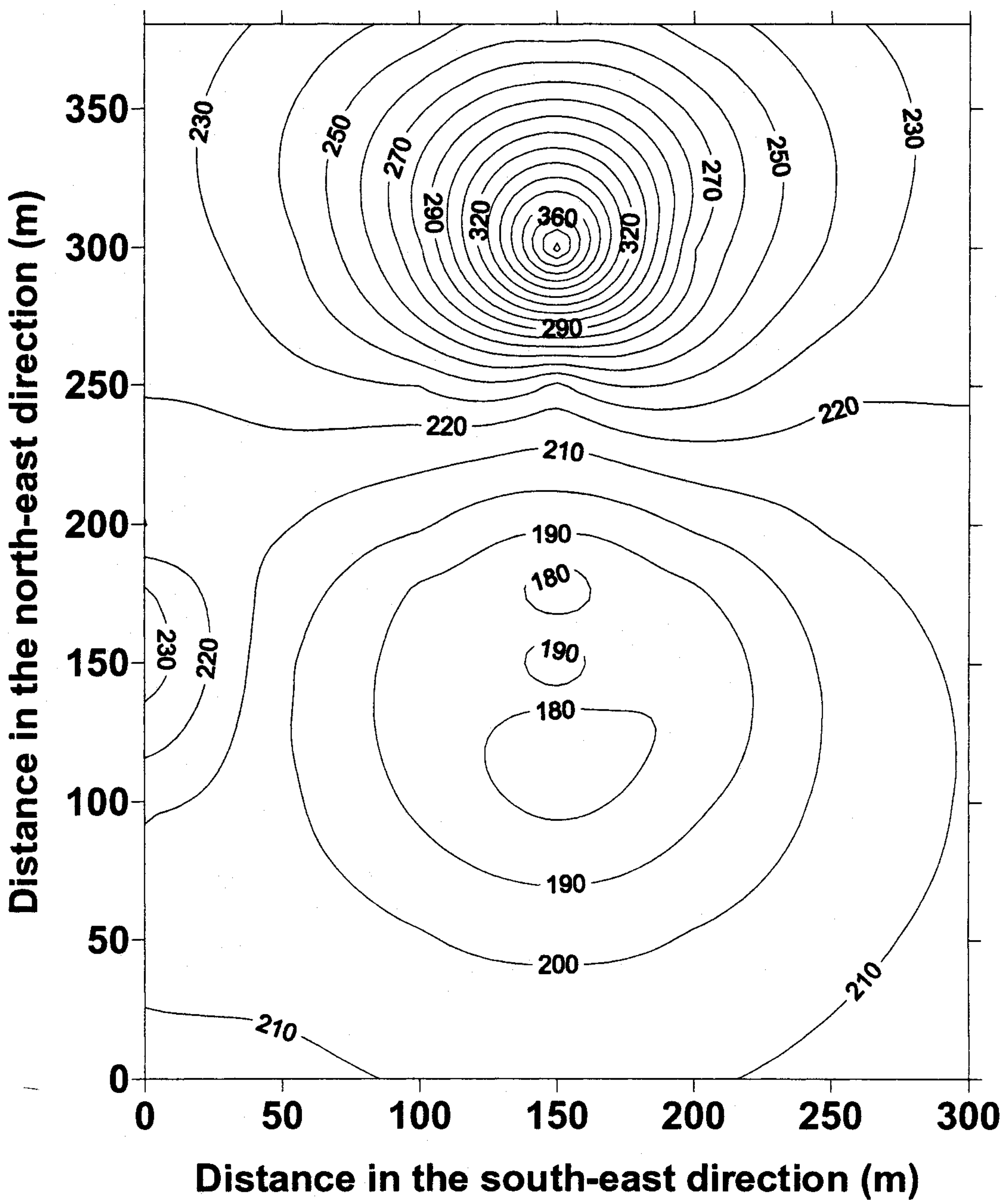


Figure 5.28 The estimated hydraulic conductivity distribution in a field problem (m/day). This figure is used in the validation of the stochastic analysis program–Case 2.

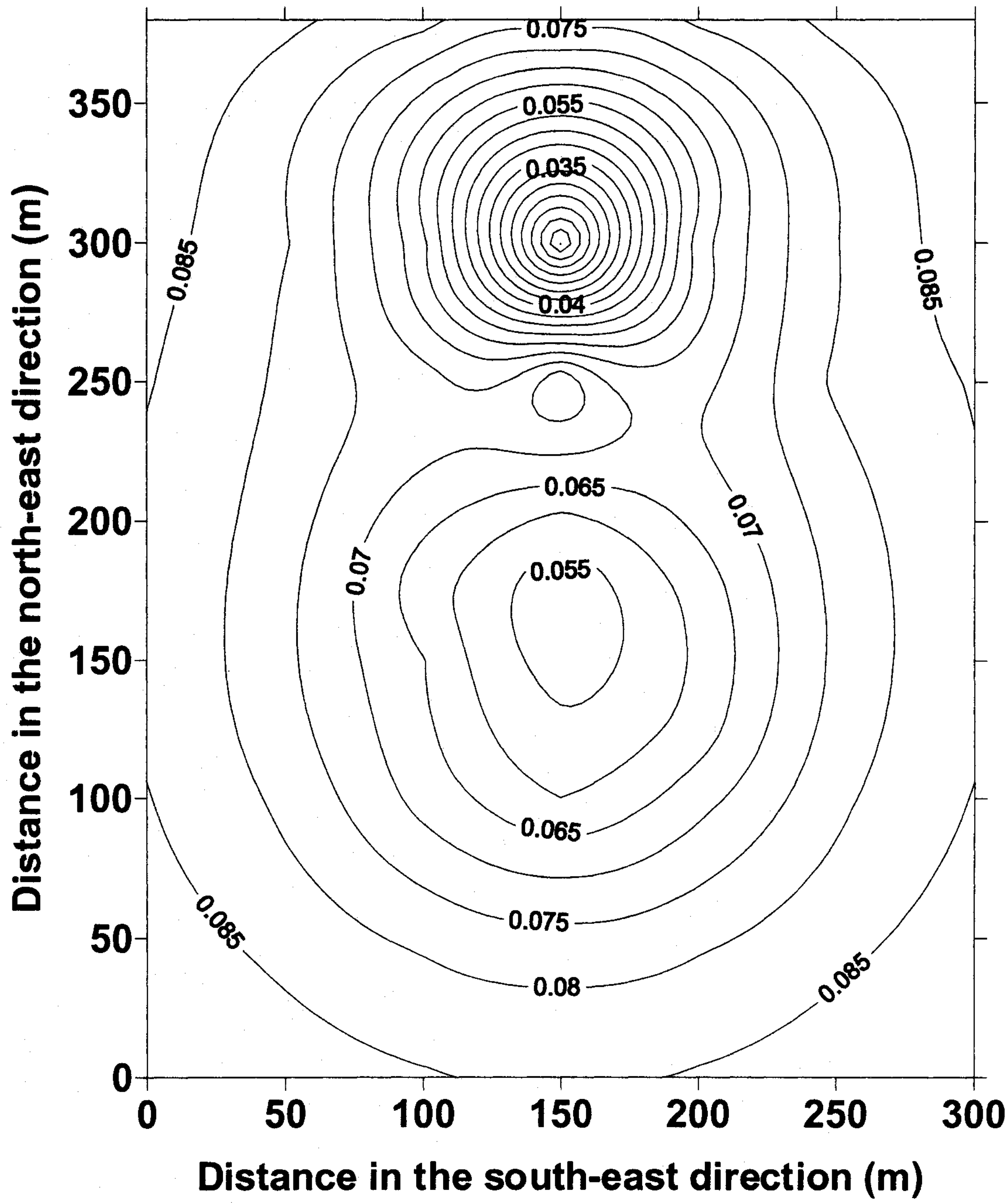


Figure 5.29 The variance distribution of the logarithm of hydraulic conductivity. This figure is used in the validation of the stochastic analysis program–Case 2

CHAPTER 6

SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS FOR FUTURE RESEARCH

6.1 Summary

Many researchers used stochastic methods in the inverse analysis of groundwater flow problems. For the solution of complex problems, numerical methods such as the finite difference or finite element method are used. Appropriate software is required for the numerical analysis. Unfortunately, such software that can be used to solve stochastic problems of groundwater flow, especially in the case of transient flow, is rare or maybe unavailable commercially. Therefore, it is necessary to develop a computer program for this purpose.

In the present study, a stochastic finite element program for inverse analysis is developed to estimate the hydraulic conductivity distribution in an area by utilizing observed data of hydraulic heads at different times and hydraulic conductivities at several observation wells. The program is based on the adjoint state method. The resulting adjoint states and expected hydraulic heads are used to calculate the covariance matrices between hydraulic heads at different times, and cross-covariance between hydraulic heads at different times and hydraulic conductivity values at different locations. The estimated statistical parameters are obtained by the MLE method. The hydraulic conductivity distribution in the aquifer is then calculated using the cokriging method. In the calculations, the logarithmic values of hydraulic conductivity are used.

An attempt has been made in this thesis to verify and validate the computer program. In the verification stage, the distribution of hydraulic conductivities in two hypothetical problems is compared to the distribution of the "true" values of hydraulic conductivities calculated by a random number generator and the Turning Band methods. Moreover, a regression analysis is performed to show the correlation between the observed and calculated values of hydraulic conductivities. For the validation of the program, two field problems are analyzed.

This software will mainly be used as a research tool and possibly to solve real field problems in the future after the analysis of a sufficient number of verification and validation problems.

6.2 Conclusions

A stochastic finite element program, STOCKINV, for inverse analysis has been developed, and therefore, the main objective of this thesis, as stated in Chapter 1, has been achieved. From the experience gained during the verification and validation of the program, the following conclusions are drawn.

- The stochastic program provides an estimate of the "true" values of the distribution of hydraulic conductivity in a confined aquifer. Estimated values compare well with true values especially at locations around the observation wells. At points significantly away from the observation wells, the correlation between the true and estimated values of hydraulic conductivity is weak. However, better estimates would probably be obtained when the number of observation wells increases and the location of wells spread evenly through out the aquifer.
- The application of the stochastic inverse analysis method to two field problems suggests that it maybe possible to extend the method to real life problems to estimate the distribution of hydraulic conductivity values.
- The stochastic finite element program can produce an estimate of the distribution of hydraulic conductivity in an area with limited observed data. Even in the

extreme case, such as the second field problem, the method was able to produce estimated values of hydraulic conductivity. As a general rule, however, the reliability of the estimated hydraulic conductivity values would reduce as the available field data become smaller.

- In this study, the available field data was limited and it was not enough to argue convincingly that the validation was complete.
- Zonation used in the analysis of inverse problems may have some effect on the estimated distribution of hydraulic conductivities in the aquifers. The effect of zonation is strong when the field data is very limited.
- The adjoint states method used in the program is an efficient method in terms of computer storage requirement and computational time. This conclusion has been made before by Sun and Yeh (1985, 1992) and Yeh (1986).
- The program can be used only for an aquifer with one type of heterogeneous material.

6.3 Recommendations for Future Research

- In this thesis, the stochastic inverse analysis is used to obtain hydraulic conductivity distribution in an aquifer. Only the hydraulic conductivities and hydraulic heads in the aquifer are considered random variables. Another parameter that appears in the governing equation of groundwater flow is the coefficient of storage. In addition, some other variables, such as the boundary conditions, the amount of recharge or discharge, are involved in the solution of the groundwater flow problems. It was assumed in the present study that these parameter and variables have constant values in the deterministic sense. Thus, it is possible to improve the program so that it can be used to estimate the distribution of hydraulic conductivity as well as the distribution of storage coefficient by considering that both parameters are random variables. Moreover, the program can be improved further by considering the boundary conditions and/or the amount of recharge or discharge as random variables.

- Contaminant transport in porous media is an important issue in groundwater management problems. In the contaminant transport calculations, both the groundwater flow equation and the hydrodynamic dispersion equation have to be solved. The groundwater flow parameters and the dispersion coefficient are required for the analysis. Therefore, it is possible to improve the method used in this thesis to study the phenomena of contaminant transport in aquifers by considering that all groundwater flow and transport parameters are random variables.

- The program, STOCHINV, is developed to estimate the hydraulic conductivity distribution in two-dimensional study domains. In a real life situation, an aquifer is always a three-dimensional geologic structure. Consequently, it is not possible to use the program when the flow through an aquifer cannot be idealized as a two-dimensional problem. Therefore, it is necessary to improve the program for modeling three-dimensional groundwater flow in aquifers.

- The program is validated utilizing observed data from two aquifers. The data is provided in two published reports. In these reports, the total number of pumping tests and observation wells was small and the wells were not spread evenly throughout the aquifers. It would be desirable to validate the program further by using data from well-instrumented aquifers in which the wells are spread evenly throughout the aquifers.

- The program, STOCHINV, is developed to estimate the hydraulic conductivity distribution in confined aquifers. In nature, there are many unconfined aquifer. For the analysis of unconfined aquifers, the program needs to be modified.

- The effect of zonation on the estimated values of hydraulic conductivities needs to be investigated.

BIBLIOGRAPHY

Abdin, A.E.A. (1996), Stochastic Analysis of Multiphase Flow in Heterogeneous Porous Media, a Ph.D. dissertation, Utah State University, Logan, Utah.

Adamowski, K. and Hamory, T. (1983), A Stochastic Systems Model of Groundwater Model Fluctuations, Journal of Hydrology, Vol. 62, pp. 129-141.

Ahlstrom, S., Foote, H., Arnett, R., Cole, C., and Serne, R. (1977), Multicomponent Mass Transport model: Theory and Numerical Implementation, Rep. BNWL 2127, Battele Pac, Northwest Lab., Richland, Wash.

The American Society for Testing and Materials (1993), 1993 Annual Book of ASTM Standards, ASTM, Philadelphia.

Amoozegar-Fard, A., Nielsen, D.R., and Warrick, A.W. (1982), Soil Solute Concentration Distribution for Spatially Varying Pore Water Velocities and Apparent Diffusion Coefficients, Soil Sci. Soc. Amer. J., Vol. 46 No. 1, pp. 3-9.

Bakr, A.A. (1976), Stochastic Analysis of the Effects of Spatial Variations of Hydraulic Conductivity of Groundwater Flow, Ph. D. Dissertation, New Mexico Institute of Mining and Technology, Socorro.

Bakr, A.A., Gelhar, L.W., Gutjhar, A.L., and MacMillan, J.R. (1978), Stochastic Analysis of Spatial Variability in Subsurface Flows, 1, Comparison of One and Three-Dimensional Flows, Water Resources Research Vol. 14, No. 2, pp. 263-272.

Bathe, K-J. (1996), Finite Element Procedures, Prentice-Hall, Englewood Cliffs, New Jersey.

Bear, J. (1979), Hydraulics of Groundwater, McGraw-Hill Inc., Tel Aviv.

Bear, J. and Verruijt, A. (1987), Modeling Groundwater Flow and Pollution, D. Reidel Publishing Company, Dordrecht, Holland.

Brassington, R. (1998), Field Hydrogeology, John Wiley and Sons Ltd, Chi Chester, England.

Carrera, J. (1984), Estimation of Aquifer Parameters under Transient and Steady State Conditions, a Ph.D. Thesis, The University of Arizona.

Carrera, J. and Neuman, S.P. (1986), Estimation of Aquifer Parameters under Transient and Steady State Conditions: 2, Uniqueness, Stability, and Solution Algorithms, Water Resources Research, Vol. 22, No. 2, pp. 211-227.

Carrera, J. (1988), State of Art of the Inverse Problem Applied to the Flow and Solute Transport Equations, in Groundwater Flow and Quality Modeling, NATO ASI Series, edited by Curtodio, E. et al., Hingham, Massachusetts.

Chankong, V. and Haimes, Y.Y. (1983), Multiobjective Decision-Making: Theory and Methodology, North-Holland, Amsterdam.

Chow, V.T., Maidment, D.R., and Mays, L.W. (1988), Applied Hydrology, McGraw-Hill Publishing Company, New York.

Dagan, G. (1982a), Stochastic Modeling of Groundwater Flow by Unconditional and Conditional Probabilities, 1, Conditional Simulation and the Direct Problem, Water Resources Research Vol. 18, No. 4, pp. 813-833.

Dagan, G. (1982b), Stochastic Modeling of Groundwater Flow by Unconditional and Conditional Probabilities, 2, The Solute Transport, Water Resources Research Vol. 18, No. 4, pp. 835-848.

Dagan, G. (1984), Solute Transport in heterogeneous Formation, J. Fluid Mech., Vol. 145, pp. 151-177.

Dagan, G. (1985), Stochastic Modeling of Groundwater flow by Unconditional and Conditional Probabilities: the Inverse Problem, Water Resources Research Vol. 21, No. 1, pp. 65-72.

Dagan, G. (1986), Statistical theory of Groundwater Flow and Transport: pore to Laboratory, laboratory to Formation, and Formation to Regional Scale, Water Resources Research, Vol. 22, No. 9, pp. 120S.

Dagan, G. (1987), The Theory of Solute Transport by Groundwater, Ann. Rev. Fluid Mech., Vol. 19, pp. 183-215.

Dagan, G. and Rubin, Y. (1988), Stochastic Identification of Recharge, Transmissivity, and Storativity in Aquifer Transient Flow: A Quasi-steady Approach, Water Resources Research, Vol. 2, No. 10, pp. 1698-1710.

Dagan, G. (1997), Stochastic Modeling of Flow and Transport: the Broad Perspective, in Subsurface Flow and Transport: A Stochastic Approach, Editors. Dagan, G. and Neuman, S.P., Cambridge University Press, Cambridge, U.K.

Dagan, G. (2002), An Overview of Stochastic Modeling of Groundwater Flow and Transport: From Theory to Applications. EOS, Transactions, American Geophysical Union Magazine. Vol. 83, No. 53, Pp. 621, 622, and 625.

Davis, J.C. (2002), Statistics and Data Analysis in Geology, John Willey and Sons, New York.

Dawson, K.J. and Istok, J.D. (1991), Aquifer Testing: Design and Analysis of Pumping and Slug Test, Lewis Publishers, Inc., Chelsea, Michigan.

de Marsily, G. (1986), Quantitative Hydrogeology, Academic Press, Inc., San Diego, California.

de Marsily, G., Combes, P., and Goblet, P. (1992), Comment on 'Groundwater Model cannot be Validated', by L.F. Konikow and J.D. Bredehoef, Advances in Water Resources Vol. 15, pp. 367-369.

Di Federico, V. and Neuman, S.P. (1998), Transport in Multiscale Log Conductivity Fields with Truncated Power Variograms, Water Resources Research, Vol. 34, No. 5, pp. 963-973.

Dogrul, E.C., Kavvas, M.L., and Chen, Z. (1998), Prediction of Subsurface Storm flow in Heterogeneous Sloping Aquifers, Journal of Hydrologic Engineering, October, pp. 258-267.

Elfeki, A.M.M. (1998), Stochastic Characterization of Geological Heterogeneity and Its Impact on Groundwater Contaminant Transport, a Ph.D. thesis, Delft University of Technology, Den Haag, A.A. Balkema, Rotterdam.

Emsellem, Y. and de Marsily, G. (1971), An Automatic Solution for the Inverse Problem, Water Resources Research, Vol. 7, No. 5, pp. 1264-1283.

Espinoza, C.A. (1997), Stochastic Analysis of the Transport of Adsorbing Pollutants in Aquifers Having Spatially Variable Chemical Properties, a Ph.D. thesis, University of Illinois at Urbana-Champaign.

Fetter, C.W. (1994), Applied Hydrogeology, 3rd ed. Prentice-Hall, Inc., Upper Saddle River, New Jersey.

Fetter, C. W. (1999), Contaminant Hydrogeology, 2nd ed. Prentice-Hall, Inc., Upper Saddle River, New Jersey.

Flavelle, P. (1992), A Quantitative Measure of Model Validation and Its Potential Use for Regulatory Purposes, Advance in Water Resources, Vol. 15, pp. 5-13.

Fletcher, R. (1999), Practical Methods of Optimization, 2nd edition. John Wiley and Sons, Cornwall, U.K.

Fox, C. (1950), An Introduction to Calculus of Variation, Oxford University Press, London, England.

Freeze, R.A. (1975), A Stochastic-Conceptual Analysis of One-Dimensional Groundwater Flow in Non Uniform Homogeneous Media, Water Resources Research, Vol. 11, No. 5, pp. 725-741.

Freeze, R.A., & Cherry, J.A. (1979), Groundwater, Prentice-Hall, Inc., Englewood Cliffs, New Jersey.

Fredlund, D.G. and Rahardjo, H. (1993), Soil Mechanics for Unsaturated Soils, John Wiley and Sons, Inc., New York.

Frind, E.O. and Pinder, G.F. (1973), Galerkin Solution of the Inverse Problem for Aquifer Transmissivity, Water Resources Research, Vol. 9, No. 5, pp. 1397-1411.

Gelfand, I.M. and Fomin, S.V. (1963), Calculus of Variation, Prentice-Hall, Inc., Englewood Cliffs, New Jersey.

Gelhar, L.W. (1976), The Effects of Hydraulic Conductivity Variations on Groundwater Flows, 2nd International Symposium on Stochastic Hydraulics, Lund, Sweden.

Gelhar, L.W., Gutjahr, A.L., and Naff, R.L. (1979), Stochastic Analysis of Macrodispersion in Stratified Aquifer, Water Resources Research, Vol. 15, No. 6, pp. 1387-1397.

Gelhar, L.W. and Axness, C.L. (1983), Three Dimensional Stochastic Analysis of Macrodispersion in Aquifers , Water Resources Research, Vol. 19, No. 1, pp. 161-180.

Gelhar, L.W., Wierenga, P.J., Rehfeldt, K.R., Duffy, C.J., Simonett, M.J., Yeh, T–C., and Strong, W.R. (1983), Irrigation Return Flow Water Quality Monitoring, Modeling and Variability in the Middle Rio Grande Valley, New Mexico, U. S. Environmental Protection Agency Project Report, EPA-600/S2-83-072.

Gelhar, L.W. (1986), Stochastic Subsurface Hydrology from Theory to Applications, Water Resources Research, Vol. 22, No. 9, pp. 135S-145S.

Gelhar, L.W. (1993), Stochastic Subsurface Hydrology, Prentice-Hall Inc., Englewood Cliffs, New Jersey.

Ghanem, R.G. and Spanos, P.D. (1990), Stochastic Finite Elements: A Spectral Approach, Springer-Verlag, New York.

Graham, W. and McLaughlin, D. (1989a), Stochastic Analysis of Nonstationary Subsurface Solute Transport, 1, Unconditional Moments, Water Resources Research, Vol. 25, No. 2, pp. 215-232.

Graham, W. and McLaughlin, D. (1989b), Stochastic Analysis of Nonstationary Subsurface Solute Transport, 2, Conditional Moments, Water Resources Research, Vol. 25, No. 11, pp. 2331-2355.

Graham, W. and McLaughlin, D. (1991), A Stochastic Model of Solute Transport in Groundwater: Application to Borden, Ontario, Tracer Test, Water Resources Research, Vol. 27, No. 6, pp. 1345-1359.

Graham, W. and Tankersley, C.D. (1994), Optimal Estimation of Spatial Variable Recharge and Transmissivity Fields Under Steady0State Groundwater Flow, Part 1, Theory, Journal of Hydrology, Vol. 157, pp. 247-266.

Grandin Jr., H. (1996), Fundamental of the Finite Element Method, Waveland Press Inc., Prospect Heights, Illinois.

Gutjhar, A.L., Gelhar, L.W., Bakr, A.A., and MacMillan, J.R. (1978), Stochastic Analysis of Spatial Variability in Subsurface Flows, 2, Evaluation and Application, Water Resources Research Vol. 14, No. 5, pp. 953-959.

Gutjahr, A.L. and Gelhar, L.W. (1981), Stochastic Analysis of Subsurface Flow: Infinite versus Finite Domains and Stationarity, Water Resources Research, Vol. 17, No. 2, pp. 337-350.

Hoeksema, R.J. (1984), The Geostatistical Approach to the Inverse Problem in Two – Dimensional Steady State Groundwater Modeling, a Ph.D. Thesis, The University of Iowa.

Hoeksema, R.J. and Kitanidis, P.K. (1984), An Application of the Geostatistical Approach to the Inverse Problem in Two-Dimensional Groundwater Modeling, Water Resources Research, Vol. 20, No. 7, pp. 1003-1020.

Hoeksema, R. J. and Kitanidis, P. K. (1985a), Analysis of the Spatial Structure of Properties of Selected Aquifers, Water Resources Research, Vol. 21, No. 4, pp. 563-572.

Hoeksema, R.J. and Kitanidis, P.K. (1985b), Comparison of Gaussian Conditional Mean and Kriging Estimation in The Geostatistical Solution of the Inverse Problem, Water Resources Research, Vol. 21, No. 6, pp. 825-836.

Holtz, R.D. and Kovacs, W.D. (1981), An Introduction to Geotechnical Engineering, Prentice-Hall, Englewood Cliffs, New Jersey.

Huebner, K.H., Thornton, E.A., and Byrom, T.G. (1995), The Finite Element Method for Engineers, John Wiley and Sons, Toronto.

Huyakorn, P.S. and Pinder, G.F. (1983), Computational Methods in Subsurface Flow, Academic Press, Inc., New York.

Isaaks, E.H. and Srivastava, R.M. (1989), An Introduction to Applied Geostatistics, Oxford University Press, New York.

Jackson, J.D. (1975), Classical Electrodynamics, Jon Wiley & Sons, Inc., New York.

Journel, A.B. and Huijbregts, Ch.J. (1978), Mining Geostatistics, Academic, New York, 1978.

Jury, W.A., Stolzy, L.H., and Shouse, P. (1982), A Field Test of the Transfer Function Model for Predicting Solute transport, Water Resources Research, Vol. 18, No. 2, pp. 369-375.

Jury, W.A., El Abd., H., and Resketo, R. (1986), Field Study of Napropamide Movement through Unsaturated Soil, Water Resources Research, Vol. 22, pp. 749-755.

Kaluarachchi, J.J. and Parker, J.C. (1989), An Efficient Finite Element Method for Modeling Multiphase Flow, Water Resources Research, Vol. 25, No. 1, pp. 43-54.

Kaluarachchi, J.J., Parker, J.C. and Lenhard, R.J. (1990), A Numerical Model for a Real Migration of Water and Light Hydrocarbon in Unconfined Aquifers, Advance Water Resources, 13, 29 – 40.

Kapoor, V. and Gelhar, L.W. (1994a), Transport in the Three-Dimensionally Heterogeneous Aquifers, 1, Dynamics of Concentration Fluctuations, Water Resources Research, Vol. 30, No. 6, pp. 1775-1788.

Kapoor, V. and Gelhar, L.W. (1994b), Transport in the Three-Dimensionally Heterogeneous Aquifers, 2, Predictions and Observations of Concentration Fluctuations, Water Resources Research, Vol. 30, No. 6, pp. 1789-1801.

Kitanidis, P.K., and Vomvoris, E.G. (1983), A Geostatistical Approach to the Inverse Problem in Groundwater Modeling (Steady State) and One-Dimensional Simulations, Water Resources Research, Vol. 19, No. 3, pp. 677-690.

Kitanidis, P.K., and Lane, R.W. (1984), Maximum Likelihood Parameter Estimation of Hydrologic Special Processes By Gauss-Newton, IIHR Technical Report No. 275.

Kitanidis, P.K. (1995), Quasi-linear Geostatistical Theory for Inversing, Water Resources Research, Vol. 31, No. 10, pp. 2411-2419.

Kitanidis, P.K., (1997), Introduction to Geostatistics, Cambridge University Press, New York.

Kitanidis, P.K. (1999), Generalized Covariance Functions Associated with the Laplace Equation and Their Use in Interpolation and Inverse Problems, Water Resources Research, Vol. 35, No. 5, pp. 1361-1367.

Kleiber, M. and Hien, T.D. (1992), The Stochastic Finite Element Method: Basic Perturbation Technique and Computer Implementation, John Wiley and Sons, Chi Chester, England.

Konikow, L.F. and Bredehoef, J. (1992), Groundwater cannot be Validated. Advances in Water Resources Vol. 15, Pp. 75-83.

Li, L. (1998), Stochastic Analysis of Solute Transport in Heterogeneous Aquifers Subject to Random Recharge and Contaminant Source Fields, a Ph.D. dissertation, University of Florida.

Li, L. and Graham, W.D. (1998), Stochastic Analysis of Solute Transport in Heterogeneous Aquifers Subject to Random Recharge, Journal of Hydrology, Vol. 206, pp. 16-38.

Li, X., Cescotto, S., and Thomas, H.R. (1999), Finite-Element Method for Contaminant Transport in Unsaturated Soils, Journal of Hydrologic Engineering, July, pp. 265-274.

Mantoglou, A. and Wilson, J.L.(1982), The Turning Bands Method for Simulation of Random Fields Using Line Generation by A Spectral Method, Water Resources Research, Vol. 18, No. 5, pp. 1379-1394.

Mantoglou, A. and Gelhar, L.W. (1987a), Stochastic Modeling of Large-Scale Transient Unsaturated Flow Systems, Water Resources Research, Vol. 23, No. 1, pp. 37-46.

Mantoglou, A. and Gelhar, L.W. (1987b), Capillary Tension Head Variance, Mean Soil Constant, and Effective Specific Soil Moisture Capacity of Transient Unsaturated Flow in Stratified Soils, Water Resources Research, Vol. 23, No. 1, pp. 47-56.

Mantoglou, A. and Gelhar, L.W. (1987c), Effective Hydraulic Conductivities of Transient Unsaturated Flow in Stratified Soils, Water Resources Research, Vol. 23, No. 1, pp. 57-67.

Mardyanto, M.A. and Evgin, E. (2003a), Estimation of Hydraulic Conductivity of an Area Using Stochastic Finite Element Method, Proceedings of 56th Canadian Geotechnical Conference, 4th Joint IAH-CNC/CGS Groundwater Specialty Conference, September 29-October 1, 2003 (In Press), Winnipeg, Manitoba, Canada.

Mardyanto, M.A. and Evgin, E. (2003b), A Stochastic Approach for the Identification of Hydraulic Conductivity of a Region, Environmental Informatics Archives of the Environmental International Society for Environmental Information Sciences (In Press), Saskatchewan, Regina, Canada.

Marie, J.R. and Hollett, K.J. (1996), Determination of Hydraulic Characteristics and Yield of Aquifers Underlying Vekol Valley Using Several Classical and Current Methods, Arizona, U. S. Geological Survey Water-Supply Paper 2453, USGS, Denver.

Marsden, J.E. and Tromba, A.J. (1988), Vector Calculus, W.H. Freeman and Company, New York.

Matheron, G. (1973), The Intrinsic Random Functions and Their Applications, Advance Applied Probability, Vol. 5, pp. 438-468.

McLaughlin, D.B, and Wood, E.F. (1988), A Distributed Parameter Approach for Evaluating the Accuracy of Groundwater Model Predictions, 1, Theory, Water Resources Research, Vol. 24, No. 7, pp. 1037-1047.

Mizell, S.A., Gutjahr, A.L., and Gelhar, L.W. (1982), Stochastic Analysis of Spatial Variability in Two-Dimensional Steady Groundwater Flow Assuming Stationary and Nonstationary Heads, Water Resources Research Vol. 18, No. 4, pp. 1053-1067.

Montgomery, D.C. and Peck, E.A. (1982), Introduction to Linear Regression Analysis, John Wiley and Sons, New York.

Myers, K.L. (2002), Applications of Stochastic Analysis in Surface and Groundwater Modelling, Proceedings of the 55th Canadian Geotechnical and 3rd Joint IAH-CNC and CGS Groundwater specialty Conferences, Niagara Falls, Ontario. October 2002. Pp. 1045-1051.

Neupauer, R.M. and Wilson, J.L. (2001), Adjoint-derived Location and Travel Time Probabilities for a Multidimensional Groundwater System, Water Resources Research, 38(6), 1657 - 1668.

Neuman, S.P. (1973), Calibration of Distributed Parameter Groundwater Flow Models Viewed as a Multiple-Objective Decision Process under Uncertainty, Water Resources Research, Vol. 9, No. 4, pp. 1006-1021.

Neuman, S.P. and Yakowitz, S. (1979), A Statistical Approach to the Inverse Problem of Aquifer Hydrology, 1, Theory, Water Resources Research, Vol. 15, No. 4, 845-860.

Neuman, S.P. (1980a), A Statistical Approach to the Inverse Problem of Aquifer Hydrology, 3, Improved Solution Method and Added Perspective, Water Resources Research, Vol. 16, No. 2, pp. 331-346.

Neuman, S.P. (1980b), Adjoint-State Finite Element Equations for Parameter Estimation, Proceedings of Third International Conference on Finite Elements in Water Resources, Editors: Wang, S. Y. et al., University of Mississippi, Mississippi.

Neuman, S.P. and Zhang, Y-K. (1990), A Quasilinear Theory of Non-Fickian and Fickian Subsurface Dispersion, 1, Theoretical Analysis with Application to Isotropic Media, Water Resources Research, Vol. 26, No. 5, pp. 887-902.

Neuman, S.P. (1993), Eularian-Lagrangian Theory of Transport in Space-Time Nonstationary Velocity Fields: Exact Nonlocal Formalism by Conditional Moments and Weak Approximations, Water Resources Research, Vol. 29, No. 3, pp. 633-645.

Pinder, G.F. and Gray, W.G. (1977), Finite Element Simulation in Surface and Subsurface Hydrology, Academic Press, London, England.

Poeter, E.P. and Hill, M.C. (1998), Documentation of UCODE, A Computer Code for Numerical Inverse Modeling, U. S. Geological Survey Water Resources Investigations Report 98-4080, Denver, Colorado.

Polmann, D.J., McLaughlin, D., Luis, S., Gelhar, L.W. and Ababou, R. (1991), Stochastic Modeling of Large-Scale Flow in Heterogeneous Unsaturated Soils, Water Resources Research, Vol. 27, No. 7, pp. 1447-1458.

Rao, C.R. (1973), Linear Statistical Inference and Its Applications, John Wiley & Sons, New York.

Rayner, J.N. (1971), An Introduction to Spectral Analysis, Pion Limited, London, England.

Richard, F.A. (2002), The Effect of Transient Flow on Contaminant Dispersion in Porous Media, Ph.D. Thesis, Ottawa-Carleton Geoscience Centre, University of Ottawa, Ottawa, Ontario, Canada.

Robin, M.J.L., Gutjahr, A.L., Sudicky, E.A., and Wilson, J.L. (1991), Spatial Variability of Strontium Distribution Coefficients and Their Correlation with Hydraulic Conductivity in the Canadian Forces Base Borden Aquifer, Water Resources Research, Vol. 27, No. 10, pp. 2619-2632.

Robin, M.J.L., Gutjahr, A.L., Sudicky, E.A., and Wilson, J.L. (1993), Cross-Correlated Random Field Generation With the Direct Fourier Transform Method, Water Resources Research, Vol. 29, No. 7, pp. 2385-2397.

Robin, M.J.L. (2002), Theory of Flow and Transport in Porous Media, a course note of GEO 5148 (67.548) course given in the Department of Earth Sciences, Faculty of Science, University of Ottawa.

Rubin, Y. and Bellin, A. (1994), Effects of Recharge on Flow Nonuniformity and Macrodispersion, Water Resources Research, Vol. 30, No. 4, pp. 939-948.

Rubin, Y. and Dagan, G. (1987a), Stochastic Identification of Transmissivity and Effective Recharge in Steady Groundwater Flow,1, Theory, Water Resources Research, Vol. 23, No. 7, pp. 1185-1192.

Rubin, Y. and Dagan, G. (1987b), Stochastic Identification of Transmissivity and Effective Recharge in Steady Groundwater Flow, 2, Case Study, Water Resources Research, Vol. 23, No. 7, pp. 1193-1200.

Rubin, Y. and Dagan, G. (1989a), Stochastic Analysis of Boundaries Effects on Head Spatial Variability in Heterogeneous Aquifers, 1, Constant Head Boundary, Water Resources Research, Vol. 24, No. 10, pp. 1689-1697.

Rubin, Y. and Dagan, G. (1989b), Stochastic Analysis of Boundaries Effects on Head Spatial Variability in Heterogeneous Aquifers, 2, Impervious Boundary, Water Resources Research, Vol. 25, No. 4, pp. 707-712.

Rutulis, M. (1977), Antler River Aquifer Investigation, Province of Manitoba, Department of Mines, Resources, and Environmental Management, Water Resources Division, Winnipeg, Manitoba.

Sagar, B. (1978), Galerkin Finite Element Procedure for Analyzing Flow through Random Media, Water Resources Research, Vol. 14, No. 6, pp. 1035-1044.

Salandin, P. and Fiorotto, V. (1998), Solute Transport in Highly Heterogeneous Aquifers, Water Resources Research, Vol. 34, No. 5, pp. 949-961.

Samper, F.J. and Neuman, S.P. (1986), Adjoint State Equations for Advective-Dispersive Transport, Sixth International Conference on Finite Elements in Water Resources, Editors: Costa, A. Sada et al., Springer-Verlag, New York.

Schweppe, F.C. (1973), Uncertain Dynamic Systems, Prentice-Hall, Inc. Englewood Cliffs, New Jersey.

Segerlind, L.J. (1976), Applied Finite Element Analysis, John Wiley and Sons, Toronto.

Shahin, M., Oorschot, H.J.L., and De Lange, S.J. (1993), Statistical Analysis in Water Resources Engineering, A. A. Balkema, Rotterdam, the Netherlands.

Smith, L. and Freeze, R.A. (1979a), Stochastic Analysis of Steady State Groundwater Flow in a Bounded Domain, 1, One-Dimensional Simulations, Water Resources Research, Vol. 15, No. 3, pp. 521-528.

Smith, L. and Freeze, R.A. (1979b), Stochastic Analysis of Steady State Groundwater Flow in a Bounded Domain, 2, Two-Dimensional Simulations, Water Resources Research, Vol. 15, No. 6, pp. 1543-1559.

Stewart, J. (1987), Calculus, Brooks/Cole Publishing Company, Belmont, California.

Sudicky, E.A. (1989), The Laplace Transform Galerkin Technique: A Time-Continuous Finite Element Theory and Application to Mass Transport in Groundwater, Water Resources Research, Vol. 25, No. 8, pp. 1833-1846.

Sun, N-Z. and Yeh, W.W-G. (1985), Identification of Parameter Structure in Groundwater Inverse Problem, Water Resources Research, Vol. 21, No. 6, pp. 869-883.

Sun, N-Z. and Yeh, W.W-G. (1990a), Coupled Inverse Problem in Groundwater Modeling, 2, Sensitivity and Parameter Identification, Water Resources Research, Vol. 26, No. 10, pp. 2507-2525.

Sun, N-Z. and Yeh, W.W-G. (1990b), Coupled Inverse Problem in Groundwater Modeling, 2, Identififiability and Experimental Design, Water Resources Research, Vol. 26, No. 10, pp. 2527-2540.

Sun, N-Z. and Yeh, W.W-G. (1992), A Stochastic Inverse Solution for Transient Groundwater Flow: Parameter Identification and Reliability Analysis, Water Resources Research, Vol. 28, No. 12, pp. 3269-3280.

Sun, N-Z. (1996), Mathematical Modeling of Groundwater Pollution, Springer-Verlag, New York Inc., New York.

Sun, N-Z. (1999), Groundwater Modeling, Kluwer Academic Publishers, Dordrecht, the Netherlands.

Sykes, J.F., Wilson, J.L. and Andrews, R.W. (1985), Sensitivity Analysis for Steady State Groundwater Flow Using Adjoint Operators, Water Resources Research, Vol. 21, No. 3, pp. 359-371.

Sykes, J.F. and Wilson, J.L. (1984), Adjoint Sensitivity Theory for the Finite Element Method, Fifth International Conference on Finite Elements in Water Resources, Editors: Liable, J. P. et al., Springer-Verlag, New York.

Tang, Y. and Aral, M.M. (1992a), Contaminant Transport in Layered Porous Media, 1, General Solution, Water Resources Research, Vol. 28, No.5, pp. 1389-1397.

Tang, Y. and Aral, M.M. (1992b), Contaminant Transport in Layered Porous Media, 2, Applications, Water Resources Research, Vol. 28, No. 5, pp. 1399-1406.

Terzaghi, K., Peck, R.B., and Masri, M.G. (1996), Soil Mechanics in Engineering Practice, John Wiley and Sons Inc., New York.

Thomas, J.R. and Finney, R.L. (1984), Calculus and Analytic Geometry, Addison-Wesley Publishing Company, Reading, Massachusetts.

Thomson, N.R. and Sykes, J.F. (1986), Numerical Aspects of Adjoint Solutions, Sixth International Conference on Finite Elements in Water Resources, Editors: Costa, A. Sada et al., Springer-Verlag, New York.

Todd, D.K. (1980), Groundwater Hydrology, John Wiley & Sons, New York.

Tompson, A.F.B., Ababou, R., and Gelhar, L.W. (1989), Implementation of the Three-Dimensional Turning Bands Random Field Generator, Water Resources Research, Vol. 25, No. 10, pp. 2227-2243.

Townley, L.R. and Wilson, J.L. (1985), Computationally Efficient Algorithms for Parameter Estimation and Uncertainty Propagation in Numerical Models of Groundwater Flow, Water Resources Research, Vol. 21, No. 12, pp. 1851-1860.

Valocchi, A. and Quinodez, A.M. (1989), Application of the Random Walk Method to Simulate the Transport of Kinetically Adsorbing Solutes, Groundwater Contamination, IAHS Publ., Vol. 185, pp. 35-42.

Vulikh, B.Z. (1963), Introduction to Functional Analysis for Scientists and Technologists, Pergamon Press, New York.

Wagner, B.J. and Gorelick, S.M. (1989), Reliable Aquifer Remediation in the Presence of Spatially Variable Hydraulic Conductivity: From data to Design, Water Resources Research, Vol. 25, No. 10, pp. 2211-2225.

Wang, H.F. and Anderson, M.P. (1982), Introduction to Groundwater Modeling: Finite Difference and Finite Element Methods, W.H. Freeman and Company, San Francisco.

Warren, J.E. and Price, H.S. (1961), Flow in Heterogeneous Porous Media, Soc. Petrol. Eng. J., Vol. 1, pp. 153-169.

Wong, H.S-T. (1998), Uncertainty Analysis in Contaminated Aquifer Management Using Mixed Monte Carlo Simulation and Gaussian Quadrature Approximation, a Ph.D. dissertation, University of California, Los Angeles.

Wood, B.D. and Kavvas, M. L. (1999), Stochastic Solute Transport under Unsteady Flow Conditions: Comparison of Theory, Monte Carlo Simulations, and Field Data, Water Resources Research, Vol. 35, No. 7, pp. 2069-2084.

Yeh, W.W-G. and Yoon, Y.S. (1981), Aquifer Parameter Identification with Optimum Dimension in Parameterization, Resources Research, Vol. 17, No. 3, pp. 664-672.

Yeh, W.W-G., Yoon, Y.S., and Lee, K.S. (1983), Aquifer Parameter Identification With Kriging and Optimum Parameterization, Water Resources Research, Vol. 19, No. 1, pp. 225-233.

Yeh, T-C., Gelhar, L.W., and Gutjahr, A.L. (1985a), Stochastic Analysis of Unsaturated Flow in Heterogeneous Soils, 2: Statistical Anisotropic Media with Variable Alpha, Water Resources Research, Vol. 21, No. 4, pp. 457-464.

Yeh, T-C., Gelhar, L.W., and Gutjahr, A.L. (1985b), Stochastic Analysis of Unsaturated Flow in Heterogeneous Soils, 3: Observations and Applications, Water Resources Research, Vol. 21, No. 4, pp. 465-471.

Yeh, W.W-G. (1986), Review of Parameter Identification Procedures in Groundwater Hydrology: The Inverse Problem, Water Resources Research, Vol. 22, No. 2, pp. 95-108.

Yeh, W.W-G., and Sun, N-Z. (1990), Variational Sensitivity Analysis, Data Requirements, and Parameter identification in a Leaky Aquifer System, Water Resources Research, Vol. 26, No. 9, pp. 1927-1938.

Yeh, T.-C. Jim, Minghui, J., and Hanna, S. (1996), An Iterative Stochastic Inverse Method: Conditional Effective Transmissivity and Hydraulic Head Field, Water Resources Research, Vol. 32, No. 1, pp. 85-92.

Zhang, D. and Neuman, S.P. (1995a), Eularian-Lagrangian Analysis of Transport Conditioned on Hydraulic Data, 1, Analytical-Numerical Approach, Water Resources Research, Vol. 26, No. 5, pp. 39-51.

Zhang, D. and Neuman, S.P. (1995b), Eularian-Lagrangian Analysis of Transport Conditioned on Hydraulic Data, 2, Effects of Log Transmissivity and Hydraulic Head Measurements, Water Resources Research, Vol. 31, No. 1, pp. 53-63.

Zhang, D. and Neuman, S.P. (1995c), Eularian-Lagrangian Analysis of Transport Conditioned on Hydraulic Data, 3, Spatial Moments, Travel Time Distribution, Mass Flow Rate, and Cumulative Release Across a Compliance Surface, Water Resources Research, Vol. 31, No. 1, pp. 65-75.

Zhang, D. and Neuman, S.P. (1995d), Eularian-Lagrangian Analysis of Transport Conditioned on Hydraulic Data, 4, Uncertain Initial Plume State and Non-Gaussian Velocities, Water Resources Research, Vol. 31, No. 1, pp. 77-88.

Zhang, D. and Winter, C.L. (1998), Nonstationary Stochastic Analysis of Steady Flow Through Variably Saturated, Heterogeneous Media, Water Resources Research, Vol. 34, No. 5, pp. 1091-1100.

Zhang, D. (2002), Stochastic Methods for Flow in Porous Media, Academic Press, Cornwall, U.K.

Zhang, Y-K. and Neuman, S.P. (1990), A Quasi-linear Theory of Non-Fickian and Fickian Subsurface Dispersion, 2, Application to Anisotropic Media and the Borden Site, Water Resources Research, Vol. 31, No. 1, pp. 903-913.

APPENDIX A

DERIVATION OF STOCHASTIC PARTIAL DIFFERENTIAL EQUATIONS

Two-dimensional groundwater flow in a heterogeneous-isotropic confined aquifer is governed by the following equation (Bear, 1979),

$$S\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x}\left(Kb\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(Kb\frac{\partial \phi}{\partial y}\right) + Q \tag{A1}$$

The solution of Eq. (A1) requires the initial and boundary conditions

$$\phi(x,y,t) = g_0;(x,y) \in (R); t = t_0 \tag{A2}$$

$$\phi|_{(\Gamma_1)} = g_1 \; ; \qquad \left(Kb\frac{\partial \phi}{\partial x} + Kb\frac{\partial \phi}{\partial y}\right).n|_{\Gamma 2} = g_2 \tag{A3}$$

where

S = coefficient of storage (dimensionless)
ϕ = hydraulic head (length)
K = hydraulic conductivity (length/time)
Q = source or sink (volume/time/area)
b = thickness of the aquifer (length)
x, y = Cartesian coordinates (length)
g_o = given functions defined on sections of flow region (R)
g_1, g_2 = given functions defined on parts of boundary (Γ_1, Γ_2)
R = the flow region
Γ_1, Γ_2= parts of boundary of the flow region (R)

n = unit vector in the direction normal to Γ_2
t = time (T)
t_0 = the initial time (T)

In the stochastic analysis, random variables Y and ϕ can be expressed as follows.

$$Y = F + f \ ; \qquad \phi = H + h \tag{A4}$$

where

F = expected value of Y, E[Y]
H = expected value of ϕ, E[ϕ]
f = the variation of Y about the mean value
h = the variation of ϕ about the mean value

Substituting Eq. (A4) into Eq. (A1) yields

$$S\frac{\partial(H+h)}{\partial t} = \frac{\partial}{\partial x}\left[e^{F+f} b \frac{\partial(H+h)}{\partial x}\right] + \frac{\partial}{\partial y}\left(e^{F+f} b \frac{\partial(H+h)}{\partial y}\right) + Q \tag{A5}$$

Each part in Eq. (A5) can be broken down into the following equations.

(i) $S\frac{\partial(H+h)}{\partial t} = S\frac{\partial H}{\partial t} + S\frac{\partial h}{\partial t}$

(ii) $$\frac{\partial}{\partial x}\left[e^{F+f} b \frac{\partial(H+h)}{\partial x}\right] = e^{F+f}\frac{\partial}{\partial x}\left(b\frac{\partial(H+h)}{\partial x}\right) + b\frac{\partial(H+h)}{\partial x}\frac{\partial\left(e^{F+f}\right)}{\partial x}$$

$$= e^{F+f}\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right) + \frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)\right] + b\frac{\partial(H+h)}{\partial x} e^{F+f}\frac{\partial(F+f)}{\partial x}$$

$$= e^{F+f}\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right) + \frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)\right]$$

$$+ be^{F+f}\left(\frac{\partial F}{\partial x}\frac{\partial H}{\partial x} + \frac{\partial f}{\partial x}\frac{\partial H}{\partial x} + \frac{\partial h}{\partial x}\frac{\partial F}{\partial x} + \frac{\partial h}{\partial x}\frac{\partial f}{\partial x}\right)$$

(iii) $\frac{\partial}{\partial y}\left[e^{F+f} b \frac{\partial (H+h)}{\partial y}\right] =$

$$e^{F+f}\left[\frac{\partial}{\partial y}\left(b\frac{\partial (H)}{\partial y}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial (h)}{\partial y}\right)\right]$$

$$+be^{F+f}\left(\frac{\partial F}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial h}{\partial y}\frac{\partial F}{\partial y}+\frac{\partial h}{\partial y}\frac{\partial f}{\partial y}\right)$$

Substitute (i), (ii), and (iii) into Eq. (A5). Similar to Sun and Yeh (1992), ignore

$$\frac{\partial h \partial f}{\partial x \partial x} \text{ and } \frac{\partial h \partial f}{\partial y \partial y} \tag{A6}$$

due to the smallness of these terms. The derivations lead to the following equation.

$$S\frac{\partial H}{\partial t}+S\frac{\partial h}{\partial t}=e^{F+f}\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right]$$
$$+be^{F+f}\left(\frac{\partial F}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial h}{\partial x}\frac{\partial F}{\partial x}+\frac{\partial F}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial h}{\partial y}\frac{\partial F}{\partial y}\right)+Q \tag{A7}$$

Dividing Eq. (A7) by e^{F+f}, the following equation can be obtained.

$$e^{-F-f}\left(S\frac{\partial H}{\partial t}+S\frac{\partial h}{\partial t}\right)=\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right]$$
$$+b\left(\frac{\partial F}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial h}{\partial x}\frac{\partial F}{\partial x}+\frac{\partial F}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial h}{\partial y}\frac{\partial F}{\partial y}\right)+e^{-F-f}Q \tag{A8}$$

Again, due to the smallness of f, exp(-f) can be approximated by (1-f) (Gutjahr and Gelhar, 1981; Dagan, 1982; Mizell et al., 1982; Hoeksema and Kitanidis, 1985b; and Sun and Yeh, 1992). Then the following equation can be obtained.

$$e^{-F}\left(S\frac{\partial H}{\partial t}+S\frac{\partial h}{\partial t}\right)-e^{-F}f\left(S\frac{\partial H}{\partial t}+S\frac{\partial h}{\partial t}\right)=\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)$$
$$+\frac{\partial}{\partial y}\left(b\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)+b\left(\frac{\partial F}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial h}{\partial x}\frac{\partial F}{\partial x}\right)$$
$$+b\left(\frac{\partial F}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial h}{\partial y}\frac{\partial F}{\partial y}\right)+e^{-F}Q-e^{-F}fQ \quad \text{(A9)}$$

Rearrange Eq. (A9), and ignore the term $f\frac{\partial h}{\partial t}$ due to its smallness. Then divide the resulting equation by e^{-F}, which yields

$$e^{F}\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)\right]+e^{F}\left[\frac{\partial}{\partial y}\left(b\frac{\partial H}{\partial y}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right]$$
$$+be^{F}\left(\frac{\partial F}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial h}{\partial x}\frac{\partial F}{\partial x}\right)+b.e^{F}\left(\frac{\partial F}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}+\frac{\partial h}{\partial y}\frac{\partial F}{\partial y}\right) \quad \text{(A10)}$$
$$+Q-fQ-S\frac{\partial H}{\partial t}-S\frac{\partial h}{\partial t}+fS\frac{\partial H}{\partial t}=0$$

Taking expectation of Eq. (A10), a stochastic partial differential equation, SPDE, for the expected H can be obtained as follows

$$S\frac{\partial H}{\partial t}=e^{F}\left[\frac{\partial}{\partial x}\left(b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial H}{\partial y}\right)\right]+Q \quad \text{(A11)}$$

Subtracting Eq. (A11) from Eq. (A10) an SPDE for f and h are obtained as follows.

$$S\frac{\partial h}{\partial t}=e^{F}\left[\frac{\partial}{\partial x}\left(b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial h}{\partial y}\right)\right]$$
$$+be^{F}\left(\frac{\partial f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial f}{\partial y}\frac{\partial H}{\partial y}\right)+f\left(S\frac{\partial H}{\partial t}-Q\right) \quad \text{(A12)}$$

In Eqs. (A11) and (A12), the terms $\frac{\partial F}{\partial x}$ and $\frac{\partial F}{\partial y}$ are equal to each other because isotropy is assumed for the hydraulic conductivity in the aquifer. In addition, it is also assumed that the logarithm of K field is statistically homogeneous, which means F is constant. As a result, $\partial F/\partial x$ and $\partial F/\partial y$ are equal to zero (see Sun, 1999).

Assuming f and h to be unknown and S to be known, the variational version of Eq. (A12) becomes

$$S\frac{\partial \delta h}{\partial t} = e^F\left[\frac{\partial}{\partial x}\left(b\frac{\partial \delta h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial \delta h}{\partial y}\right)\right]$$

$$+be^F\left(\frac{\partial \delta f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial \delta f}{\partial y}\frac{\partial H}{\partial y}\right)+\delta f\left(S\frac{\partial H}{\partial t}-Q\right) \tag{A13}$$

The initial and boundary conditions are

$$\delta h|_{t=0} = 0; (x,y)\in(R) \tag{A14a}$$

$$\delta h|_{\Gamma_1} = 0; \qquad e^F\left(\frac{\partial \delta h}{\partial x}+\frac{\partial \delta h}{\partial y}\right)\cdot n|_{\Gamma_2} = 0 \tag{A14b}$$

Multiplying Eq. (A13) by an arbitrary function ψ and integrating over (R) x (0, T) yields

$$\int_0^T\int_R \psi\left\{S\frac{\partial \delta h}{\partial t} - e^F\left[\frac{\partial}{\partial x}\left(b\frac{\partial \delta h}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial \delta h}{\partial y}\right)\right]\right\}dRdt$$

$$-\int_0^T\int_R \psi\left\{be^F\left(\frac{\partial \delta f}{\partial x}\frac{\partial H}{\partial x}+\frac{\partial \delta f}{\partial y}\frac{\partial H}{\partial y}\right)+\delta f\left(S\frac{\partial H}{\partial t}-Q\right)\right\}dRdt = 0 \tag{A15}$$

The following conditions can be assumed.

$$\psi(x,y,t)=0;(x,y)\in(R);t=t_0 \tag{A16a}$$

$$\psi\big|_{\Gamma_1}=0; \qquad e^F\left(\frac{\partial\psi}{\partial x}+\frac{\partial\psi}{\partial y}\right)\cdot n\,\big|_{\Gamma 2}=0 \tag{A16b}$$

Using Green's identities to exchange ψ and δf and δh yields

(1) $\int_0^T\int_R \psi S\frac{\partial\delta h}{\partial t}dRdt=\int_R \psi S\delta h\Big|_0^T dR-\int_0^T\int_R \delta hS\frac{\partial\psi}{\partial t}dRdt$

(2) $\int_R \psi\frac{\partial}{\partial x}\left(b\frac{\partial\delta h}{\partial x}\right)dR=\int_R \delta h\frac{\partial}{\partial x}\left(b\frac{\partial\psi}{\partial x}\right)dR-\int_\Gamma b\left(\psi\frac{\partial\delta h}{\partial x}-\delta h\frac{\partial\psi}{\partial x}\right)\cdot nd\Gamma$

(3) $\int_R \psi b\frac{\partial\delta f\partial H}{\partial x\partial x}dR=-\int_R \delta f\frac{\partial}{\partial x}\left(\psi b\frac{\partial H}{\partial x}\right)dR+\int_\Gamma \delta f.b\psi\frac{\partial H}{\partial x}\cdot nd\Gamma$

The same procedure can be applied for the space variable y.
Substitution of (1) – (3) for x and y space variables into Eq. (A15) yields

$$\int_R \psi S\delta h\Big|_0^T dR-\int_0^T\int_R \delta hS\frac{\partial\psi}{\partial t}dRdt-\int_0^T\int_R e^F\left\{\delta h\frac{\partial}{\partial x}\left(b\frac{\partial\psi}{\partial x}\right)+\delta h\frac{\partial}{\partial y}\left(b\frac{\partial\psi}{\partial y}\right)\right\}dRdt$$
$$-\quad+\int_0^T\int_R e^F\left\{\delta f\frac{\partial}{\partial x}\left(\psi b\frac{\partial H}{\partial x}\right)+\delta f\frac{\partial}{\partial y}\left(\psi b\frac{\partial H}{\partial y}\right)\right\}dRdt-\int_0^T\int_R \delta f\psi\left(S\frac{\partial H}{\partial t}-Q\right)dRdt$$
$$-\int_\Gamma e^F\left\{b\left(\psi\frac{\partial\delta h}{\partial x}-\delta h\frac{\partial\psi}{\partial x}\right)-b\left(\psi\frac{\partial\delta h}{\partial y}-\delta h\frac{\partial\psi}{\partial y}\right)\right\}.nd\Gamma$$
$$-\int_0^T\int_\Gamma e^F\left\{\left(\delta f.b\psi\frac{\partial H}{\partial x}\right)+\left(\delta f.b\psi\frac{\partial H}{\partial y}\right)\right\}\cdot nd\Gamma=0 \tag{A17}$$

Because of the initial and boundary conditions of Eqs. (A14a), (A14b), (A16a) and (A16b), the first term on the left hand side and all integral terms along the surface (Γ) vanish and Eq. (A17) becomes

$$\int_0^T\int_R\left\{S\frac{\partial\psi}{\partial t}+e^F\left[\frac{\partial}{\partial x}\left(b\frac{\partial\psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial\psi}{\partial y}\right)\right]\right\}\delta h dRdt$$

$$+\int_0^T\int_R\left\{e^F\left[-\frac{\partial}{\partial x}\left(\psi b\frac{\partial H}{\partial x}\right)-\frac{\partial}{\partial y}\left(\psi b\frac{\partial H}{\partial y}\right)\right]+\psi\left(S\frac{\partial H}{\partial t}-Q\right)\right\}\delta f dRdt=0 \quad \text{(A18)}$$

The objective function can be chosen as the following equation

$$\Omega(h,f)=\int_0^T\int_R G(h,f;x,t)dRdt \quad \text{(A19)}$$

where T is a given time and G is a user-chosen function.

The variation of performance function Ω is

$$\delta\Omega=\int_0^T\int_R\left(\frac{\partial G}{\partial h}\delta h+\frac{\partial G}{\partial f}\delta f\right)dRdt \quad \text{(A20)}$$

Because ψ is an arbitrary function (Neuman, 1980a, 1980b; Carrera and Neuman, 1986; Sun and Yeh, 1992), it can be chosen so that the terms which contain the unknown δh vanish. Select ψ in (R) x (0,T) so that it satisfies the following equation

$$\frac{\partial G}{\partial h}=S\frac{\partial\psi}{\partial t}+e^F\left[\frac{\partial}{\partial x}\left(b\frac{\partial\psi}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial\psi}{\partial y}\right)\right] \quad \text{(A21)}$$

After subtracting Eq. (A18) from Eq. (A20) and substituting Eq. (A11) into the resulting equation, the integral associated with δh vanishes and the following equation is obtained.

$$\delta\Omega=\int_0^T\int_R\left\{\frac{\partial G}{\partial f}+e^F\left[\frac{\partial}{\partial x}\left(\psi b\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(\psi b\frac{\partial H}{\partial y}\right)\right]-\psi\left(S\frac{\partial H}{\partial t}-Q\right)\right\}\delta f dRdt \quad \text{(A22)}$$

The functional derivative of Eq. (A22) is

$$\frac{\partial \Omega}{\partial f} = \int_0^T \int_R \left\{ \frac{\partial G}{\partial f} + e^F \left[\frac{\partial}{\partial x}\left(\psi b \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y}(\psi b \frac{\partial H}{\partial y}) \right] - \psi \left(S \frac{\partial H}{\partial t} - Q \right) \right\} dRdt \qquad \text{(A23)}$$

The second and third terms of the right hand side of Eq. (A23) can be expressed as

$$\frac{\partial}{\partial x}\left(\psi b \frac{\partial H}{\partial x} \right) = b \frac{\partial \psi}{\partial x}\frac{\partial H}{\partial x} + \psi \frac{\partial}{\partial x} b \frac{\partial H}{\partial x} \qquad \text{(A24a)}$$

$$\frac{\partial}{\partial y}\left(\psi b \frac{\partial H}{\partial y} \right) = b \frac{\partial \psi}{\partial y}\frac{\partial H}{\partial y} + \psi \frac{\partial}{\partial y}\left(b \frac{\partial H}{\partial y} \right) \qquad \text{(A24b)}$$

Therefore, using Eq. (3.7) in Eq. (A23) yields

$$\frac{\partial \Omega}{\partial f} = \int_0^T \int_R \left\{ \frac{\partial G}{\partial f} + e^F b \left[\frac{\partial \psi}{\partial x}\frac{\partial H}{\partial x} + \frac{\partial \psi}{\partial y}\frac{\partial H}{\partial y} \right] \right\} dRdt \qquad \text{(A25)}$$

Equation (A25) is the same equation as Eq. (3.13).

However, to calculate all elements in the Jacobian, Eq. (3.13) needs to be modified as follows.

Substitution of Eq. (3.15) into Eq. (3.10) leads to

$$\Omega = \int_0^T \int_R h(x,t) \delta(x - x_l) \delta(t - t_p) dRdt = \int_0^T \int_R h(x_l, t_p) dRdt \qquad \text{(A26)}$$

At the right hand side of Eqs. (3.13) and (A25), there is a term $\frac{\partial G}{\partial f}$. Since G is independent of f, then this term vanishes.

Substitute Eq. (A26) into the left hand side of Eq. (3.13), then the left hand side of Eq. (3.13) becomes.

$$\frac{\partial \Omega}{\partial f} = \frac{d}{df} \int_0^T \int_R h(x_l, t_p) dR dt \tag{A27}$$

The Liebnitz' rule as written in Eq. (A28) can be used to transform Eq. (A27) into Eq. (A29) as follows.

$$\frac{d}{dx} \int_{a(x)}^{b(x)} f(x,t) dy = \int_{a(x)}^{b(x)} \frac{\partial f(x,y)}{\partial t} dy + f[x, b(x)] \frac{db}{dx} - f[x, a(x)] \frac{da}{dx} \tag{A28}$$

Equation (A29) is obtained when the second and third terms on the right-hand side of Eq. (A28) vanish since time, T, and space, R, are not a function of f.

$$\frac{d}{df} \int_0^T \int_R h(x_l, t_p) dR dt = \int_0^t \int_R \frac{\partial h(x_l, t_p)}{\partial f} dR dt \tag{A29}$$

After differentiating both sides of Eq. (A29) with respect to both R and T, the following equation is obtained.

$$\frac{\partial h(x_l, t_p)}{\partial f} = \frac{\partial h(x_l, t_p)}{\partial f} \tag{A30}$$

Substituting Eq. (A30) into Eq. (3.13) leads to Eq. (3.16).

APPENDIX B

DERIVATION OF STOCHASTIC FINITE ELEMENT EQUATIONS

In the finite element analysis using the Galerkin method, an approximate or trial solution of the expected hydraulic head $\hat{H}$ can be expressed as a summation of products of nodal hydraulic heads, H_L, and the weighted average in terms of basis functions, $\zeta_L(x,y)$ (Wang and Anderson, 1982); i.e.

$$\hat{H}(x,y) = \sum_{L=1}^{NNODE} H_L \zeta_L(x,y) \qquad \text{(B1)}$$

where subscript L is nodal number and NNODE is the total number of nodal points in the problem domain. In order to solve Eq. (3.7) for the expected head, H, both sides of this equation are multiplied by the basis function first. Then, integration is performed over the entire domain.

$$\iint_R \left\{ e^F \left[\frac{\partial}{\partial x}\left(b\frac{\partial \hat{H}}{\partial x}\right) + \frac{\partial}{\partial y}\left(b\frac{\partial \hat{H}}{\partial y}\right)\right] + Q - \left(S\frac{\partial \hat{H}}{\partial t}\right)\right\} \zeta_L(x,y)\,dxdy = 0 \qquad \text{(B2)}$$

Applying the Green's identity, yields

$$\iint_R e^F b\left[\frac{\partial \zeta_L}{\partial x}\frac{\partial \hat{H}}{\partial x}+\frac{\partial \zeta_L}{\partial y}\frac{\partial \hat{H}}{\partial y}\right]dxdy = \iint_R Q\zeta_L(x,y)dx,dy$$

$$-\iint_R\left(S\frac{\partial \hat{H}}{\partial t}\right)\zeta_L(x,y)dxdy + e^F b\int_\Gamma\left\{\frac{\partial \hat{H}}{\partial x}n_x+\frac{\partial \hat{H}}{\partial y}n_y\right\}\zeta_L(x,y)d\Gamma \quad \text{(B3)}$$

where

R = the study domain
L = the nodal points
ζ(x,y) = the basis function
Γ = the surface of the domain where the specified flow is given

The integral term along the boundary Γ is set to be zero since along the boundary the hydraulic heads are specified.

A linear interpolation within a triangular element, as shown in Figure 4.1, can be expressed as

$$\hat{H}^{el}(x,y) = a_0 + a_1 x + a_2 y \quad \text{(B4a)}$$

H values at the nodal points are then written as follows.

$$H_i = a_0 + a_1 x_i + a_2 y_i \quad \text{(B4b)}$$

$$H_j = a_0 + a_1 x_j + a_2 y_j \quad \text{(B4c)}$$

$$H_k = a_0 + a_1 x_k + a_2 y_k \quad \text{(B4d)}$$

where H_m (where m = i, j, k) denotes nodal hydraulic heads and subscripts i, j, k denote nodal points of triangular elements; a_0, a_1, a_2 are constants that require to be found; and the superscript el denotes the element under consideration.

Solving Eq. (B4b), (B4c) and (B4d) for a_0, a_1, a_2 and substituting back into Eq. (B4a) the following equation is obtained

$$\hat{H}^{el}(x,y)=\zeta_i^{el}(x,y)H_i(t)+\zeta_j^{el}(x,y)H_j(t)+\zeta_k^{el}(x,y)H_k(t) \tag{B5a}$$

where

$$\zeta_i^{el}(x,y)=\frac{1}{2A^{el}}\left[(x_j y_k - x_k y_j)+(y_j - y_k)x+(x_k - x_j)y\right] \tag{B5b}$$

$$\zeta_j^{el}(x,y)=\frac{1}{2A^{el}}\left[(x_k y_i - x_i y_k)+(y_k - y_i)x+(x_i - x_k)y\right] \tag{B5c}$$

$$\zeta_k^{el}(x,y)=\frac{1}{2A^{el}}\left[(x_i y_j - x_j y_i)+(y_i - y_j)x+(x_j - x_i)y\right] \tag{B5d}$$

$$2A^{el}=(x_i y_j - x_j y_i)+(x_k y_i - x_i y_k)+(x_j y_k - x_k y_j) \tag{B5e}$$

where

A^{el} = the area of triangle

ζ_m^{el} = the element interpolation or basis function

Evaluating Eq. (B3) element by element and rearranging the resulting equation, yields

$$\sum_{el}\left\{\iint_{el} e^F b\left[\frac{\partial \zeta_L}{\partial x}\frac{\partial \hat{H}^{el}}{\partial x}+\frac{\partial \zeta_L}{\partial y}\frac{\partial \hat{H}^{el}}{\partial y}+\right]\right\}dxdy+\sum_{el}\iint_{el}\left(S\frac{\partial \hat{H}^{el}}{\partial t}\right)\zeta_L(x,y)dxdy$$

$$=\sum_{el}\iint_{el} Q\zeta_L(x,y)dxdy \tag{B6}$$

where L = 1, 2, …, NNODE

The derivative of nodal hydraulic heads can be written in terms of nodal hydraulic head values times the derivative of element basis functions as follows

$$\frac{\partial \hat{H}^{el}}{\partial x} = \frac{\partial \zeta_i^{el}}{\partial x} H_i + \frac{\partial \zeta_j^{el}}{\partial x} H_j + \frac{\partial \zeta_k^{el}}{\partial x} H_k \tag{B6a}$$

$$\frac{\partial \hat{H}^{el}}{\partial y} = \frac{\partial \zeta_i^{el}}{\partial y} H_i + \frac{\partial \zeta_j^{el}}{\partial y} H_j + \frac{\partial \zeta_k^{el}}{\partial y} H_k \tag{B6b}$$

The basis functions are linear in x and y; therefore, the gradients $\frac{\partial \hat{H}^{el}}{\partial x}$ and $\frac{\partial \hat{H}^{el}}{\partial y}$ are constant within the element as shown in Eqs. (B6a) and (B6b). The results of the integration become the integrand times the area of the element. Consequently, the first and second terms in brackets of Eq. (B6) can be expressed as

$$\iint_{el} \left(\frac{\partial \zeta_L}{\partial x} \frac{\partial \hat{H}^{el}}{\partial x} + \frac{\partial \zeta_L}{\partial x} \frac{\partial \hat{H}^{el}}{\partial y} \right) dxdy = A^{el} \left(\frac{\partial \zeta_L^{el}}{\partial x} \frac{\partial \zeta_i^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y} \frac{\partial \zeta_i^{el}}{\partial y} \right) H_i$$

$$+ A^{el} \left(\frac{\partial \zeta_L^{el}}{\partial x} \frac{\partial \zeta_j^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y} \frac{\partial \zeta_j^{el}}{\partial y} \right) H_j + \left(\frac{\partial \zeta_L^{el}}{\partial x} \frac{\partial \zeta_k^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y} \frac{\partial \zeta_k^{el}}{\partial y} \right) H_k \tag{B7}$$

where L = i, j, k.

The derivative of the expected head H in Eq. (B3) with respect to time can also be expressed in terms of basis functions by

$$\frac{\partial \hat{H}^{el}}{\partial t} = \zeta_i^{el}(x,y) \frac{\partial H_i}{\partial t} + \zeta_j^{el}(x,y) \frac{\partial H_j}{\partial t} + \zeta_k^{el}(x,y) \frac{\partial H_k}{\partial t} \tag{B8}$$

Then, the third term on the left side of Eq. (B6) can be expressed as

$$\iint_{el} S \frac{\partial \hat{H}^{el}}{\partial t} \zeta_L(x,y) dxdy = S \iint_{el} \zeta_i^{el} \zeta_L^{el} \frac{\partial H_i^{el}}{\partial t} dxdy$$

$$+ S \iint_{el} \zeta_j^{el} \zeta_L^{el} \frac{\partial H_j^{e}}{\partial t} dxdy + S \iint_{el} \zeta_k^{e} \zeta_L^{el} \frac{\partial H_k^{el}}{\partial t} dxdy \tag{B9}$$

The time derivative in the finite difference approach is expressed as

$$\left\{ \frac{\partial H}{\partial t} \right\} = \frac{1}{\Delta t} \left(\{h\}^{t+\Delta t} - \{h\}^{t} \right) \tag{B10}$$

where $\left\{ \frac{\partial H}{\partial t} \right\}$ is a column matrix in which each entry at node J and time t is $\frac{\partial H_L}{\partial t}$. Δt is a time step.

The approximation of time derivative at a single node J can be expressed as

$$\frac{\partial H_L}{\partial t} = \frac{H_L^{t+\Delta t} - H_L^{t}}{\Delta t} \tag{B11}$$

The term at the right hand side of Eq. (B6) that contains the source or sink term Q can be rewritten as follows

$$\sum_{el} \left\{ \iint_{el} Q \zeta_L(x,y) dxdy \right\} = \iint_{el} Q \zeta_i^{el}(x,y) dxdy$$

$$+ \iint_{el} Q \zeta_j^{el}(x,y) dxdy + \iint_{el} Q \zeta_k^{el}(x,y) dxdy \tag{B12}$$

Therefore, after involving the time in the equation, the matrix form of Eq. (B6) can be written as follows

$$[A]\{H\}^{t+\Delta t} = \{M\} + [D]\{H\}^{t} \quad \text{(B13)}$$

where

$$[A] = e^{F} b[C] + [D] \quad \text{(B14)}$$

$$[D] = \frac{1}{\Delta t}[P] \quad \text{(B15)}$$

$$C_{L,i}^{el} = A^{el}\left(\frac{\partial \zeta_L^{el}}{\partial x}\frac{\partial \zeta_i^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y}\frac{\partial \zeta_i^{el}}{\partial y}\right) \quad \text{(B16a)}$$

$$C_{L,j}^{el} = A^{el}\left(\frac{\partial \zeta_L^{el}}{\partial x}\frac{\partial \zeta_j^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y}\frac{\partial \zeta_j^{el}}{\partial y}\right) \quad \text{(B16b)}$$

$$C_{L,k}^{el} = A^{el}\left(\frac{\partial \zeta_L^{el}}{\partial x}\frac{\partial \zeta_k^{el}}{\partial x} + \frac{\partial \zeta_L^{el}}{\partial y}\frac{\partial \zeta_k^{el}}{\partial y}\right) \quad \text{(B16c)}$$

L = i, j, or k.

Matrix [C] becomes $[C]_{L,m} = \sum_{el} C_{L,m}^{el}$, for all L and m (m = i, j, k).

The amount of storage assigned to each nodal point of an element is calculated by the following equations.

$$P_{L,i}^{el} = S\iint_{el} \zeta_i^{el} \zeta_L^{el}\, dxdy \quad \text{(B17a)}$$

$$P_{L,j}^{el} = S\iint_{el} \zeta_j^{el} \zeta_L^{el} dxdy \tag{B17b}$$

$$P_{L,k}^{el} = S\iint_{el} \zeta_k^{el} \zeta_L^{el} dxdy \tag{B17c}$$

In the global sense, matrix [P] is a summation of the storage values at the nodes of all the elements in the study domain. This matrix can be expressed as follows.

$$[P]_{L,m} = \sum_{el} P_{L,m}^{el} \qquad \text{for all L and m} \tag{B17d}$$

where L = i, j, or k and m (m = i, j, k)

The nodal values of recharge and/or discharge in an element can be calculated by the equations given below.

$$M_i^{el} = \iint_{el} Q\zeta_i^{el}(x,y)dxdy = QA^{el}/3 \tag{B18a}$$

$$M_j^{el} = \iint_{el} Q\zeta_j^{el}(x,y)dxdy = QA^{el}/3 \tag{B18b}$$

$$M_k^{el} = \iint_{el} Q\zeta_k^{el}(x,y)dxdy = QA^{el}/3 \tag{B18c}$$

The recharge-discharge matrix {M} in the global coordinate system is obtained by the following equation.

$$\{M\}_L = \sum_{el} M_L^{el}, \text{ for all L (L = i, j, or k)} \tag{B18d}$$

Similar to the previous section, an approximate or trial solution of the adjoint state, $\hat{\psi}$, can be expressed as a summation of products of nodal adjoints ψ_L and the weighted average in terms of basis functions $\zeta_L(x,y)$; i.e.

$$\hat{\psi}(x,y) = \sum_{L=1}^{NNODE} \psi_L \zeta_L(x,y) \tag{B19}$$

The adjoint state in an element then can be expressed as

$$\psi^{el}(x,y) = \zeta_i^{el}(x,y)\psi_i(t) + \zeta_j^{el}(x,y)\psi_j(t) + \zeta_k^{el}(x,y)\psi_k(t) \tag{B20}$$

where ζ_i^{el}, ζ_j^{el}, and ζ_k^{el} are described at the previous section.

Before proceeding into Eq. (3.12) to obtain the adjoint state, ψ; the properties of the Dirac delta function will be written. This material is taken from Classical Electrodynamics by J. D. Jackson (1975).

In one dimension, the properties of the Dirac delta function are

(1) $\delta(x-a) = 0$ for $x \neq a$

(2) $\int \delta(x-a)dx = 1$ if the region of integration includes x = a; otherwise it is zero.

For an arbitrary function f(x), it has a property as follows.

(3) $\int f(x)\delta(x-a)dx = f(a)$

In two dimensions, with Cartesian coordinates, the Dirac delta function is expressed as follows.

(4) $\delta(x-X)=\delta(x_1-X_1)\delta(x_2-X_2)$. It is a function which vanishes everywhere except at x = X.

(5) $\int_{\Delta A}\delta(x-X)dA=1$ if ΔA contains x = X; otherwise it is zero.

Integrating Eq. (3.12) over the entire domain of the problem, then multiplying by the weighting average (i.e. basis functions) and making it equal to zero gives

$$\iint_R e^F\left\{\frac{\partial}{\partial x}\left(b\frac{\partial\hat{\psi}}{\partial x}\right)+\frac{\partial}{\partial y}\left(b\frac{\partial\hat{\psi}}{\partial y}\right)+S\left(\frac{\partial\hat{\psi}}{\partial t}\right)-\frac{\partial\hat{G}}{\partial h}\right\}\zeta_L(x,y)dxdy=0 \tag{B21}$$

Applying Green's identity yields

$$e^F b\iint_R\left\{\left(\frac{\partial\zeta_L}{\partial x}\frac{\partial\hat{\psi}}{\partial x}\right)+\left(\frac{\partial\zeta_L}{\partial y}\frac{\partial\hat{\psi}}{\partial y}\right)\right\}dxdy=\iint_R\left(S\frac{\partial\hat{\psi}}{\partial t}-\frac{\partial\hat{G}}{\partial h}\right)\zeta_L(x,y)dxdy \tag{B22}$$

Neuman (1980a) points out that the integral over Γ is equal to zero because of prescribed flux boundaries. At the nodes where heads are specified the values of adjoint states ψ equal to zero for all x ∈ R. As a consequence, there are no integral terms over the surface Γ in Eq. (B22).

Evaluating Eq. (B22) element by element yields

$$\sum_{el}e^F b\iint_{el}\left\{\left[\left(\frac{\partial\zeta_L}{\partial x}\frac{\psi^{el}}{\partial x}\right)+\left(\frac{\partial\zeta_L}{\partial y}\frac{\psi^{el}}{\partial y}\right)\right]\right\}dxdy$$

$$=\sum_{el}\iint_R\left(S\frac{\partial\hat{\psi}^{el}}{\partial t}-\frac{\partial\hat{G}^{el}}{\partial h}\right)\zeta_L(x,y)dxdy \tag{B23}$$

$$\frac{\partial \hat{\psi}^{el}}{\partial x} = \frac{\partial \zeta_i^{el}}{\partial x}\psi_i + \frac{\partial \zeta_j^{el}}{\partial x}\psi_j + \frac{\partial \zeta_k^{el}}{\partial x}\psi_k \tag{B24}$$

$$\frac{\partial \hat{\psi}^{el}}{\partial y} = \frac{\partial \zeta_i^{el}}{\partial y}\psi_i + \frac{\partial \zeta_j^{el}}{\partial y}\psi_j + \frac{\partial \zeta_k^{el}}{\partial y}\psi_k \tag{B25}$$

$$\frac{\partial \hat{\psi}^{el}}{\partial t} = \zeta_i^{el}(x,y)\frac{\partial \psi_i^{el}}{\partial t} + \zeta_j^{el}(x,y)\frac{\partial \psi_j^{el}}{\partial t} + \zeta_k^{el}(x,y)\frac{\partial \psi_k^{el}}{\partial t} \tag{B26}$$

$$\frac{\partial G^{el}}{\partial h} = \zeta_i^{el}(x,y)\frac{\partial \hat{G}_i}{\partial h} + \zeta_j^{el}(x,y)\frac{\partial \hat{G}_j}{\partial h} + \zeta_k^{el}(x,y)\frac{\partial \hat{G}_k}{\partial h} \tag{B27}$$

where

$$\frac{\partial G_i}{\partial h} = \delta(x_i - x_l)\delta(y_i - y_l)\delta(t - t_p) \tag{B27a}$$

$$\frac{\partial G_j}{\partial h} = \delta(x_j - x_l)\delta(y_j - y_l)\delta(t - t_p) \tag{B27b}$$

$$\frac{\partial G_k}{\partial h} = \delta(x_k - x_l)\delta(y_k - y_l)\delta(t - t_p) \tag{B27c}$$

Then Eq. (B27) can be rewritten as

$$\begin{aligned}\frac{\partial G^{el}}{\partial h} = {} & \zeta_i^{el}(x,y)\delta(x_i - x_l)\delta(y_i - y_l)\delta(t - t_p) \\ & + \zeta_j^{el}(x,y)\delta(x_j - x_l)\delta(y_j - y_l)\delta(t - t_p) \\ & + \zeta_k^{el}(x,y)\delta(x_k - x_l)\delta(y_k - y_l)\delta(t - t_p)\end{aligned} \tag{B28}$$

Therefore, at a point $x = x_l$,, $y = y_l$, and at the time $t = t_p$ the value of the derivative will be the basis function itself. At the other points and times the value of the derivative is zero.

Using Eqs. (B24) and (B25) in the first two terms of Eq. (B23), the following equation is obtained

$$\sum_{el}\iint_{el}\left(\frac{\partial\zeta_L}{\partial x}\frac{\partial\hat{\psi}^{el}}{\partial x}+\frac{\partial\zeta_L}{\partial y}\frac{\partial\hat{\psi}^{el}}{\partial y}\right)dxdy = A^{el}\left(\frac{\partial\zeta_L^{el}}{\partial x}\frac{\partial\zeta_i^{el}}{\partial x}+\frac{\partial\zeta_L^{el}}{\partial y}\frac{\partial\zeta_i^{el}}{\partial y}\right)\psi_i$$

$$+A^{el}\left(\frac{\partial\zeta_L^{el}}{\partial x}\frac{\partial\zeta_j^{el}}{\partial x}+\frac{\partial\zeta_L^{el}}{\partial y}\frac{\partial\zeta_j^{el}}{\partial y}\right)\psi_j+A^{el}\left(\frac{\partial\zeta_L^{el}}{\partial x}\frac{\partial\zeta_k^{el}}{\partial x}+\frac{\partial\zeta_L^{el}}{\partial y}\frac{\partial\zeta_k^{el}}{\partial y}\right)\psi_k$$

(B29)

Substitution of Eq. (B26) into the first term on the right-hand side of Eq. (B23) yields

$$\iint_{el} S\frac{\partial\hat{\psi}^{el}}{\partial t}\zeta_L(x,y)dxdy = S\iint_{el}\left(\zeta_i^{el}\zeta_L^{el}\frac{\partial\psi_i}{\partial t}+\zeta_j^{el}\zeta_L^{el}\frac{\partial\psi_j}{\partial t}+\zeta_k^{el}\zeta_L^{el}\frac{\partial\psi_k}{\partial t}\right)dxdy$$

(B30)

Substitution of Eq. (B27) into the second term on the right-hand side of Eq. (B23) yields

$$\iint_{el}\frac{\partial\hat{G}}{\partial h}\zeta_L(x,y)dxdy = \iint_{el}\left[\zeta_L^{el}\left\{\zeta_i^{el}\frac{\partial G_i}{\partial h}\right\}\right]dxdy$$

$$+\iint_{el}\left[\zeta_L^{el}\left\{\zeta_j^{el}\frac{\partial G_j}{\partial h}\right\}\right]dxdy+\iint_{el}\left[\zeta_L^{el}\left\{\zeta_k^{el}\frac{\partial G_k}{\partial h}\right\}\right]dxdy \qquad \text{(B31)}$$

Therefore, after involving the time derivative using the finite difference method, Eq. (B23) can be written in matrix form as follows

$$[A]\{\psi\}^{t+\Delta t} = [D]\{\psi\}^{t} + \{E\} \tag{B32}$$

where

$$[A] = e^{F} b[C] + [D] \tag{B33}$$

[A] is an L x L matrix.

$$E_{L,i}^{el} = \iint_{el} \zeta_i^{el} \zeta_L^{el} \frac{\partial G_i}{\partial h} dxdy \tag{B34a}$$

$$E_{L,j}^{el} = \iint_{el} \zeta_j^{el} \zeta_L^{el} \frac{\partial G_j}{\partial h} dxdy \tag{B34b}$$

$$E_{L,k}^{el} = \iint_{el} \zeta_k^{el} \zeta_L^{el} \frac{\partial G_k}{\partial h} dxdy \tag{B34c}$$

where

L = i, j, or k.

The gradient of function G in the global coordinate system, {E}, is given below.

$$\{E\}_{L,m} = \sum_{el} E_{L,m}^{el} \text{ , for all L and m (m = i, j, k)} \tag{B34d}$$

Matrices [D] and [C] were defined before in Eqs. (B14) and (B15).

Considering Eqs. (B1) and (B18), Neuman (1980b) implies that

$$\frac{\partial \Omega}{\partial f} = \frac{\partial \Omega}{\partial f_i} \zeta_i \tag{B35}$$

Utilizing Eq. (B35), Eq. (3.16) can be expressed as

$$\frac{\partial h(x_l,t_p)}{\partial f_i} = \int_0^T \int_{R_i} \left\{ e^F b \left[\frac{\partial \psi}{\partial x}\frac{\partial H}{\partial x} + \frac{\partial \psi}{\partial y}\frac{\partial H}{\partial y} \right] \right\} \zeta_i(x,y) dR dt \tag{B36}$$

After the expected heads, H, and the adjoint states, Ψ, were obtained by solving Eqs. (B12) and (B32), respectively, the results can be substituted into Eq. (B36) and the following equation is obtained (Neuman, 1980b).

$$\frac{\partial h(x_l,t_p)}{\partial f_i} = e^F B \sum_{n=1}^{NNODE} \sum_{m=1}^{NNODE} B_{inm} \sum_{p} \int_{p}^{t_{p+1}} \psi_n H_m dt \tag{B37}$$

where

$$B_{inm} = \int_R \nabla\zeta_n . \nabla\zeta_m . \zeta_i(x,y) dR \tag{B38}$$

n, m are the nodal numbers in the global coordinate system and i is the number of parameter zones.

The third summation in Eq. (B37) must be held over all time steps.

APPENDIX C

THE MAXIMUM LIKELIHOOD ESTIMATION (MLE)

The maximum likelihood estimate is a method for estimating statistical parameters that appear in Eqs. (3.1) and (3.2). The details of this method are given below.

The Gaussian joint probability function for N measurements is given by (Kitanidis, and Vomvoris, 1983; Kitanidis and Lane, 1984; Hoeksema and Kitanidis, 1984; Wagner and Gorelick, 1989) as

$$p(\underline{z}|\underline{\theta}) = (2\pi)^{-N/2} |Q|^{-1/2} \exp\left(-\frac{1}{2}(\underline{z}-\underline{\mu})^T Q^{-1} (\underline{z}-\underline{\mu})\right) \tag{C1}$$

where $\underline{z}$ is the vector of available measurements, $| \ |$ denotes determinant, $\underline{\theta}$ (σ_Y^2, μ, l_Y) is a 1-D matrix containing the statistical parameters to be determined. Q is the measurement covariance matrix given by Eqs. (3.22) or (3.23).

The parameter vector, $\underline{\theta}(\sigma_Y^2, \mu, l_Y)$, is determined using the maximum likelihood estimation or the minimization of the negative log likelihood function as follows (Kitanidis and Lane, 1984).

$$LG(\underline{z}|\underline{\theta}) = -ln\, p(\underline{z}|\underline{\theta}) = \frac{N}{2} ln(2\pi) + \frac{1}{2} ln|Q| + \frac{1}{2}(\underline{z}-\underline{\mu})^T Q^{-1} (\underline{z}-\underline{\mu}) \tag{C2}$$

The derivative of the negative log-likelihood with respect to a scalar parameter θ_j is given by

$$\frac{\partial LG}{\partial \theta_j} = \frac{1}{2} tr\left(Q^{-1} \frac{\partial Q}{\partial \theta_j} \right) - \frac{1}{2}(z-\mu)^T Q^{-1} \frac{\partial Q}{\partial \theta_j} Q^{-1}(z-\mu) - (z-\mu)^T Q^{-1} \frac{\partial \mu}{\partial \theta_j} \qquad \text{(C3)}$$

In Eq. (C3) the following relations were adopted (Schweppe, 1973).

$$\frac{\partial}{\partial \theta_j} ln|Q| = tr\left[Q^{-1} \frac{\partial Q}{\partial \theta_j} \right] \qquad \text{(C4)}$$

$$\frac{\partial}{\partial \theta_j} Q^{-1} = -Q^{-1} \frac{\partial Q}{\partial \theta_j} Q^{-1} \qquad \text{(C5)}$$

To determine the parameter vector $\underline{\theta}$ (σ_Y^2, μ, l_Y), the vector of the derivatives has to be set zero; i.e. for the gradient $g_j = \left. \frac{\partial LG}{\partial \theta_j} \right|_{\underline{\theta}=\underline{\theta}^*}$;

$$\underline{g} = 0 \qquad \text{(C6)}$$

This problem can be solved using a gradient-based iterative method with the basic iteration as follows

$$\underline{\theta}_{i+1} = \underline{\theta}_i - \rho_i R_i \underline{g}_i \qquad \text{(C7)}$$

where

θ_i = parameter vector in the i[th] iteration
ρ_i = a scalar step-size parameter that can be chosen so that $LG(z|\theta_{i+1}) \prec LG(z|\theta_i)$
$\underline{g}_i$ = the gradient vector at i

R_i = an approximation of the second derivative matrix $\left(\frac{\partial^2 LG}{\partial\theta^2}\right)^{-1}\Big|_{\theta=\theta_i}$

This method also has been known as the 'method of Scoring' or Gauss-Newton method. In this method, R_i is approximated by the inverse of the Fisher information matrix M_i^{-1}. The Fisher information matrix is given by

$$M_i = E\left\{\left(\frac{\partial^2 LG}{\partial\theta^2}\right)\Big|_{\theta=\theta_i}\right\} = E\left\{\frac{\partial LG}{\partial\theta}\left(\frac{\partial LG}{\partial\theta}\right)^T\Big|_{\theta=\theta_i}\right\} \tag{C8}$$

The (j,k) element of M_i is given by

$$M(j,k) = E\left(\frac{\partial LG}{\partial\theta_j}\frac{\partial LG}{\partial\theta_k}\right) \tag{C9}$$

Equation (C9) can be calculated by employing Gauss moment. The resulting factorization is

$$M_{jk} = \frac{1}{2}tr\left(Q^{-1}\frac{\partial Q}{\partial\theta_j}Q^{-1}\frac{\partial Q}{\partial\theta_k}\right) + \left(\frac{\partial\mu}{\partial\theta_j}\right)^T Q^{-1}\frac{\partial\mu}{\partial\theta_k} \quad \text{C10)}$$

The iteration procedure is as follows

i. Calculate the gradient vectors, g_i, and the Fisher information matrix, M_i, at all iterations.

ii. Estimate the parameters at the next iteration using the following equation

$$\underline{\theta}_{i+1} = \underline{\theta}_i - \rho_i(M_i)^{-1}\underline{g}_i \tag{C11}$$

In this iteration, as suggested by Kitanidis and Lane, 1984, ρ_i is chosen as 1.

In the matrix form, Eq. (C11) can be written as

$$\begin{Bmatrix} \theta_j \\ \cdot \\ \cdot \\ \theta_J \end{Bmatrix}_{i+1} = \begin{Bmatrix} \theta_j \\ \cdot \\ \cdot \\ \theta_J \end{Bmatrix}_i - \begin{bmatrix} M_{jk} & \dots & M_{jK} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ M_{Jk} & \dots & M_{JK} \end{bmatrix}_i^{-1} \begin{Bmatrix} g_j \\ \cdot \\ \cdot \\ g_{Jj} \end{Bmatrix}_i \tag{C12}$$

where

j = number of parameters to be estimated
i = number of iterations
jk = element number of the Fisher information matrix

For multiple parameters, the stopping criteria of the iteration is (Kitanidis and Lane, 1984)

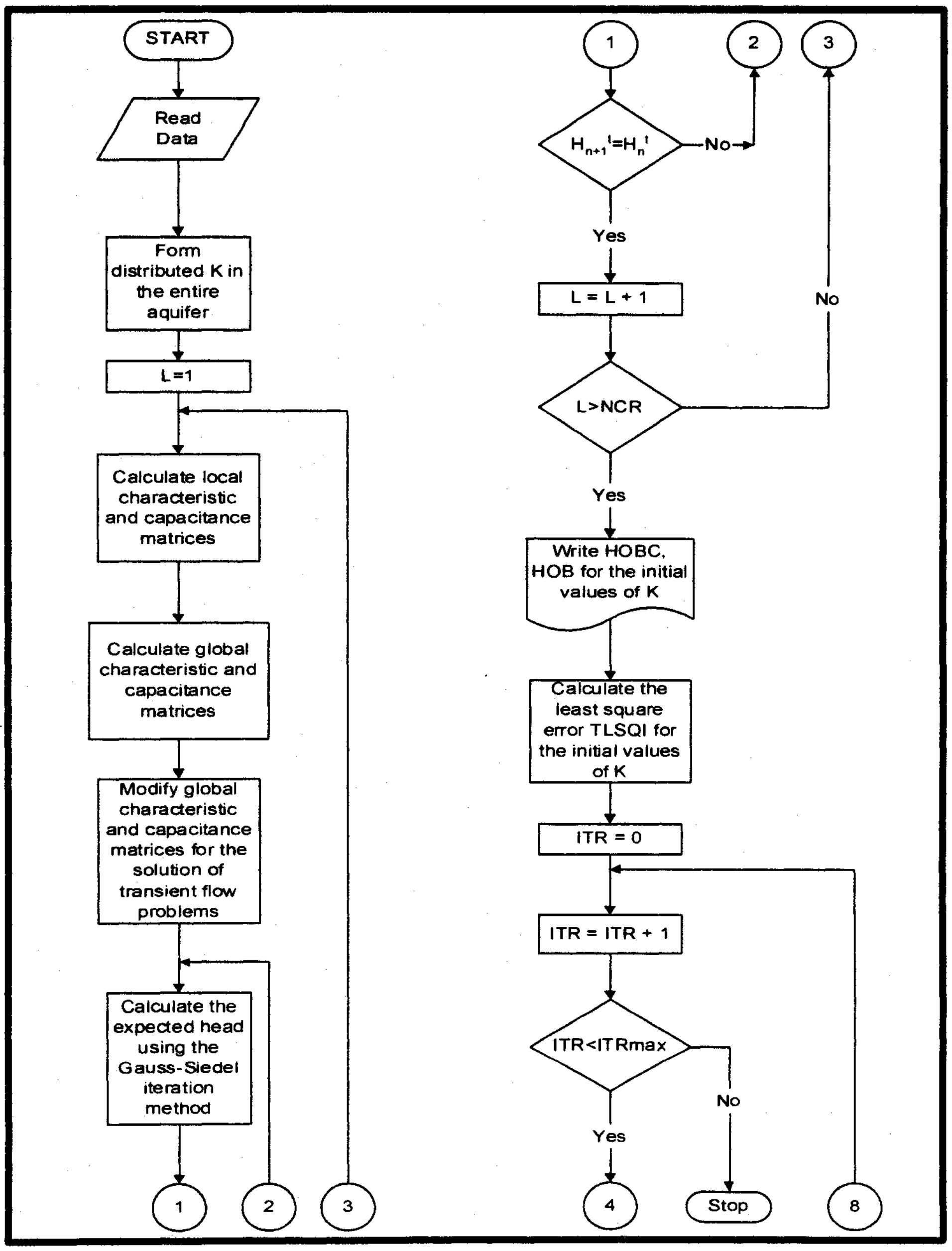
$$(\underline{\theta}_i - \underline{\theta}_{i-1})^T M (\underline{\theta}_i - \underline{\theta}_{i-1}) = 0.01 \tag{C13}$$

The details of the method of scoring can be found in Kitanidis and Lane (1984), and Rao (1973).

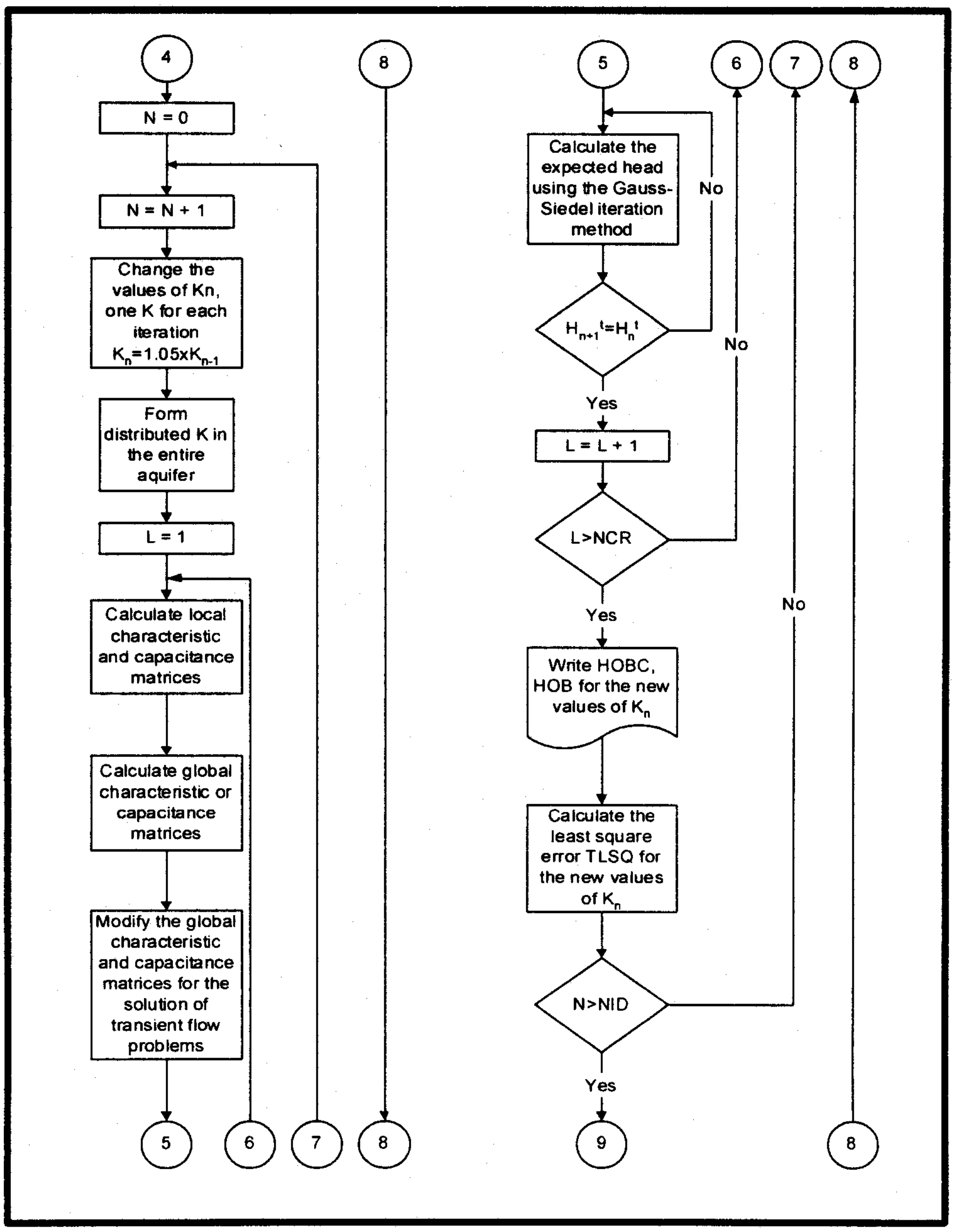
APPENDIX D

FLOWCHART OF THE COMPUTER PROGRAMS

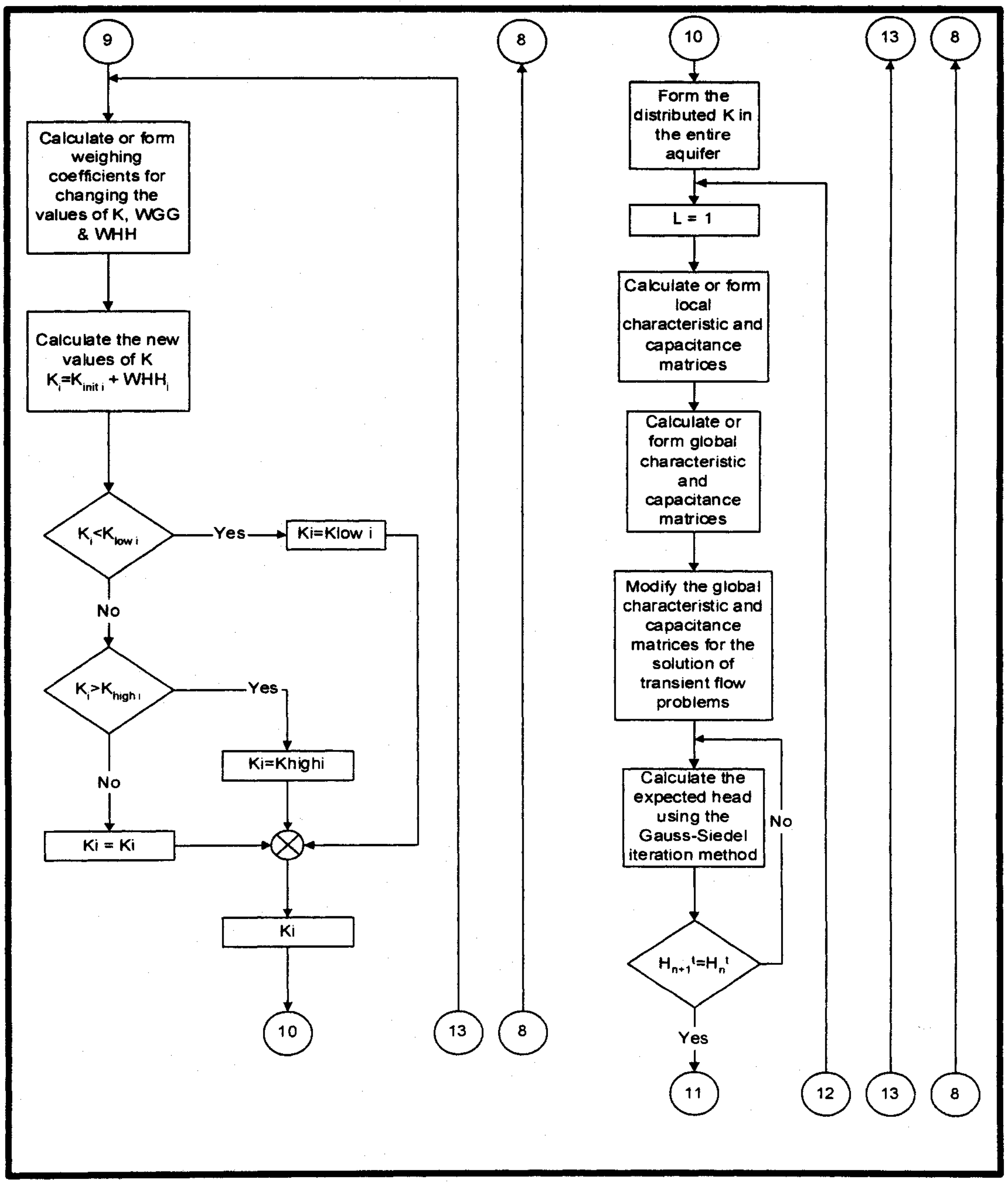
PROGRAM 1



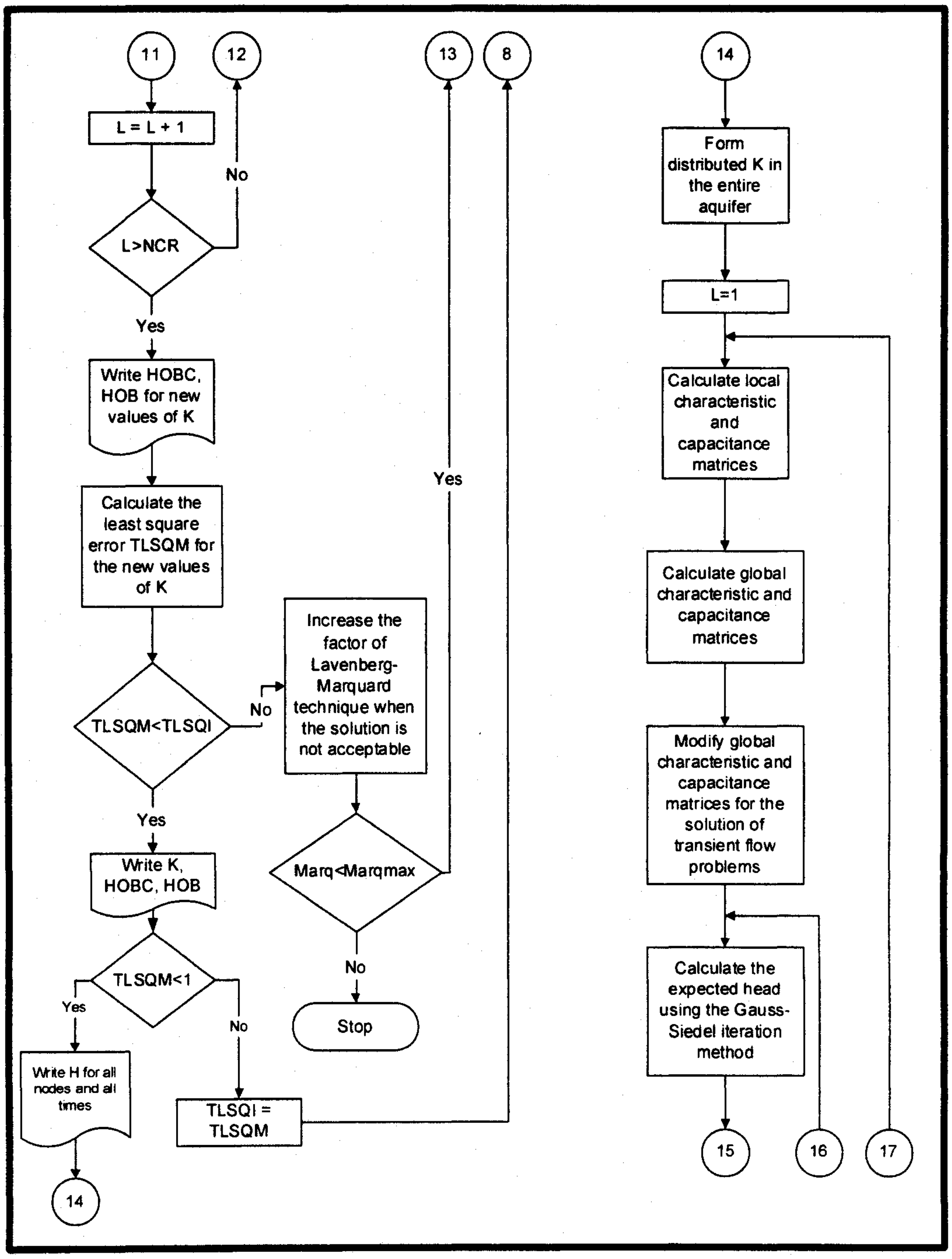
PROGRAM 1 (continue)



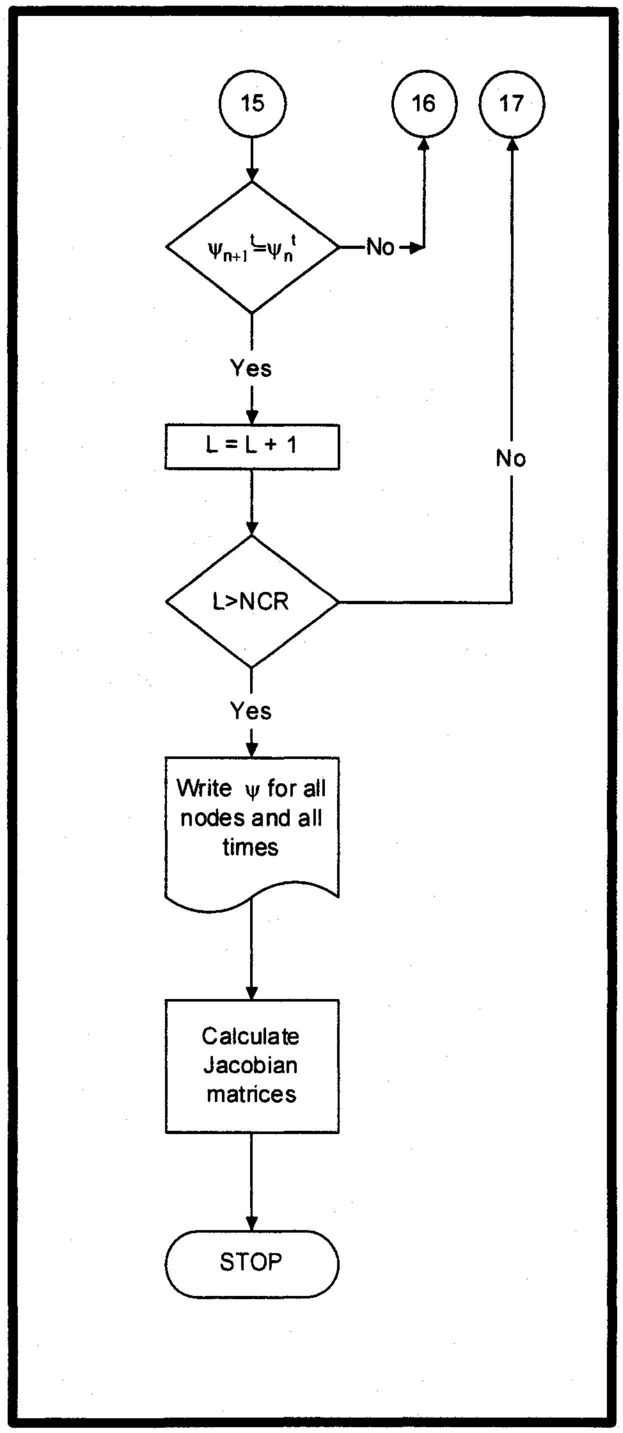
PROGRAM 1 (continue)



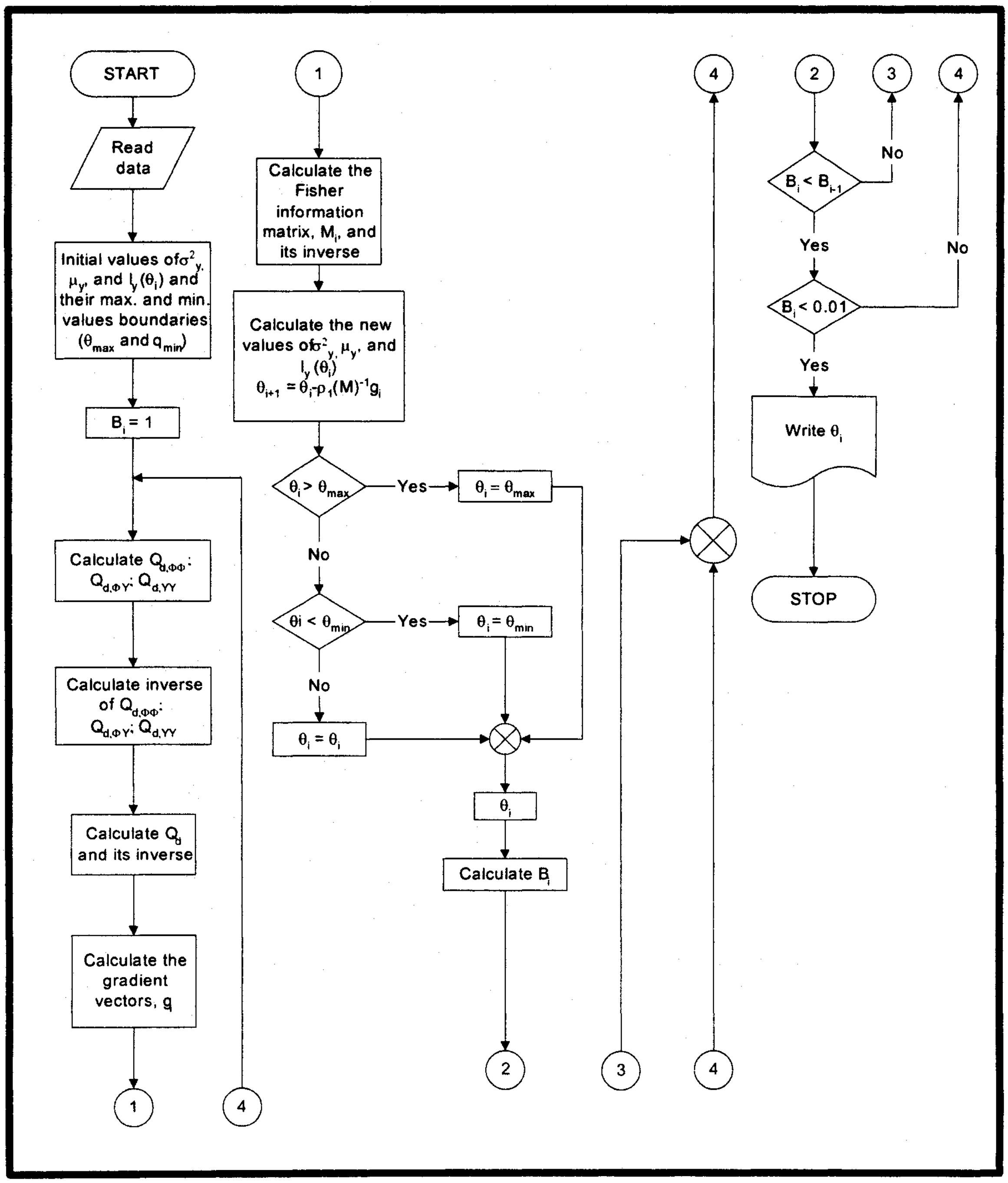
PROGRAM 1 (continue)



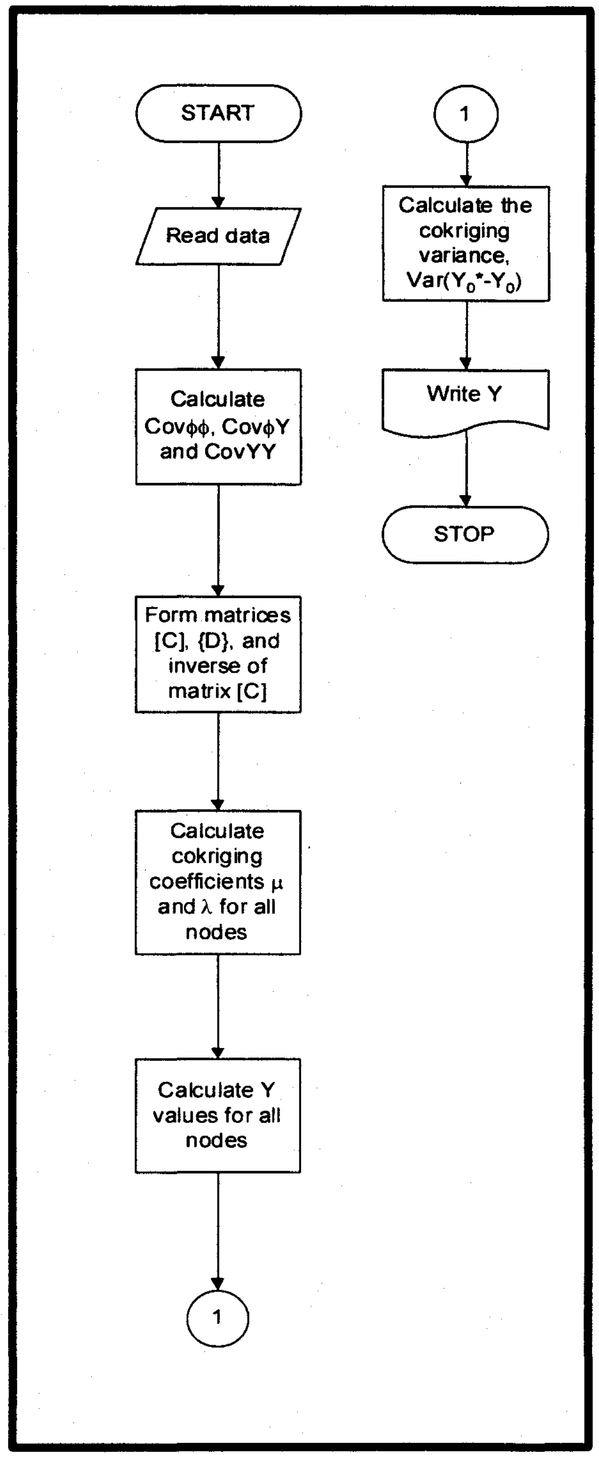
PROGRAM 1 (continue)



PROGRAM 2


START
Read data
Initial values of σ²y, μy, and Iy(θi) and their max. and min. values boundaries (θmax and qmin)
Bi = 1
Calculate Qd,ΦΦ; Qd,ΦY; Qd,YY
Calculate inverse of Qd,ΦΦ; Qd,ΦY; Qd,YY
Calculate Qd and its inverse
Calculate the gradient vectors, gi
1
4
1
Calculate the Fisher information matrix, Mi, and its inverse
Calculate the new values of σ²y, μy, and Iy (θi) θi+1 = θi-ρ1(M)-1gi
θi > θmax
Yes
θi = θmax
No
θi < θmin
Yes
θi = θmin
No
θi = θi
θi
Calculate Bi
2
3
4
4
2
3
4
Bi < Bi-1
No
Yes
Bi < 0.01
No
Yes
Write θi
STOP

PROGRAM 3


START
Read data
Calculate Covφφ, CovφY and CovYY
Form matrices [C], {D}, and inverse of matrix [C]
Calculate cokriging coefficients μ and λ for all nodes
Calculate Y values for all nodes
1
1
Calculate the cokriging variance, Var(Y0*-Y0)
Write Y
STOP

APPENDIX E

DEFINITION OF TERMS USED IN THIS THESIS

Anisotropic soil is a soil in which hydraulic conductivity values in the soil are directional dependent; i.e., Kx ≠ Ky ≠ Kz. The axes are labeled as x, y, and z in the Cartesian coordinate system. Note: in this thesis, the term anisotropy refers to hydraulic conductivity.

Autocovariance or covariance function, Cov(h), is a function that describes the relationship between the values of a random variable determined at different locations separated by a certain distance. Some times, this distance is called a lag. This relationship is a function of the distance between the points, but not the space coordinates of these points (see Robin, 2002).

$$Cov_{yy}(h) = E\left(y'(x+h)\cdot y'(x)\right) \tag{E1}$$

and it can be estimated by

$$Cov_{yy}(h) = \frac{1}{N_p}\sum_{i_p=1}^{N_p}\left[y'(x+h)\cdot y'(x)\right]_{i_p}$$

$$= \frac{1}{N_p}\sum_{i_p=1}^{N_p}\left[\left(y(x+h)-\bar{y}\right)\cdot\left(y(x)-\bar{y}\right)\right]_{i_p} \tag{E2}$$

where N_p = the number of pairs of points separated by the lag h.

h = the lag or separated distance between data points

i_p = the i^{th} pair

$y(x)$ = the value of data or parameter at location x.

$y(x+h)$ = the value of data or parameter at location x+h

$\bar{y}$ = the mean value of the realization of the data

The superscript (′) indicates the perturbation of the parameter.

Calibration is a process of adjusting model parameters such that the calculated outcome of the process is comparable to the observed result. This process is also called history matching.

Coefficient of storage/storativity is a property of soil that describes the amount of water that can be taken out from or put into storage per unit surface area per unit decline or increase of hydraulic head perpendicular to that surface.

Cokriging is similar to kriging; however, besides using the observed values of the same variable, it also uses the observed values of two (or more) variables; i.e., to estimate an unknown value of hydraulic conductivity at point x_0 by utilizing observed magnitudes of hydraulic conductivity at points $x_1, x_2, \ldots, x_n$ and observed values of hydraulic head at points $y_1, y_2, \ldots, y_m$. Both variables have to be spatially correlated.

Cross-covariance is a function that describes the relationship between two random variables. The relationship between two random variables can be in time and/ or space.

Deterministic process is a process in which all variables included in the analysis can be determined precisely. In other words, there is no random variable included in the analysis.

Disjunctive kriging is similar to kriging; nonetheless, besides estimating a magnitude at a point, in disjunctive kriging one can also estimate the probability of the estimated value whether it exceeds or is less than the 'true' value at this point.

Ensemble is "a collection of all possible realizations of a process" (Shahin et al., 1993)

Ergodicity: The term ergodicity refers to the condition in which a collection of data of a single realization can represent the ensemble or the collection of all possible realizations of a process. In this condition, the average of parameters that are obtained from a realization is similar to the average of the ensemble of data.

Expectation or expected value is also called mean value. It measures the central tendency of random variables. For a discrete random variable, the expected value can be written as

$$E(X) = \sum_{all\,x_i} x_i p_x(x_i) \tag{E3}$$

where $p_x(x_i)$ is the probability mass function and X is a discrete random variable. For a continuous random variable, the expected value can be written as

$$E(X) = \int_{-\infty}^{\infty} x f_x(x) dx \tag{E4}$$

where $f_x(x)$ is a probability density function and X is a continuous random variable.

Forward problem refers to a problem for which the governing equation is solved to obtain the dependent variables. The independent variables are provided as input. For example, hydraulic head values are calculated in a groundwater flow problem by specifying the hydraulic conductivity values and the boundary conditions as input.

Heterogeneous aquifer is an aquifer in which the hydraulic conductivity value is different at different locations. Note: in this thesis, the term heterogeneous refers to the hydraulic conductivity.

Homogeneous aquifer is an aquifer in which its hydraulic conductivity value is the same at all locations in the aquifer. Note: in this thesis, the term homogeneous refers to the hydraulic conductivity.

Hydraulic conductivity (K) provides information on how fast a fluid can move through a porous medium. The unit of K is (Length/Time).

Hydraulic head or total head in a flow through porous medium is defined as the sum of the elevation head and the piezometric head. It can be written as (Terzaghi et al., 1996)

$$\phi = z + \frac{u}{\gamma_w} \qquad \text{(E5)}$$

where

ϕ = the hydraulic head (m)

z = the elevation head (m)

u = the pore water pressure (kPa)

γ_w = the unit weight of water (kN/m^3)

$\frac{u}{\gamma_w}$ = the piezometric head (m)

The movement of water in a porous media is due to the difference between hydraulic head at different points.

Inverse problem refers to a problem for which the governing equation is solved to obtain the independent variables. The dependent variables are provided as input. For example, hydraulic conductivity values are calculated in a groundwater flow problem by using the measured hydraulic head values and the boundary conditions as input.

Isotropic soils are soils in which hydraulic conductivity values in the soils are independent of direction; i.e., Kx = Ky = Kz. Note: in this thesis, the term isotropy is used in relation to the hydraulic conductivity.

Kriging is a method to estimate an unknown or unsampled value of parameter that is distributed in space. The estimation of the unknown value utilizes the observed values of the same parameter. For example, the unknown value of the hydraulic conductivity at point, x_0, can be calculated using the observed values of hydraulic conductivity at points $x_1, x_2, \ldots, x_n$.

Perturbation is the magnitude of variation from the mean value of a collection of values related to a random variable.

P-value is defined as "the smallest level of significance at which the null hypothesis would be rejected for a specific test" (Davis, 2002).

Realization is a collection of data collected or measured at a given time.

Specific surface is "the ratio of the surface area of a material to either its mass or volume" (Holtz and Kovacs, 1981).

Specific yield (Sy) is a property of soil that describes the ratio of amount of water in a saturated soil that can be drawn by gravity to the total volume of the soil. The ratio between the amounts of water retained in the same soil to the total volume of soil is called specific retention (Sr). Therefore, the summation of Sy and Sr is the porosity of the soil (α); i.e., α = Sy + Sr.

Spectral analysis is "a procedure of calculating and interpreting a spectrum" (Rayner, 1971).

Spectrum (or spectral density function) is a function that describes the stochastic process in a frequency domain.

Stationary stochastic process refers to a process, which meets the following condition. If a set of random variables is divided into several non-overlapping sub-sets such that the mean (and maybe variance) of the random variables are the same for each sub-set, then the stochastic process is called stationary. In other words, the statistical properties of the stochastic process do not change with time or space. If both the mean and variance of each sub-set are invariant, the process is called a second order stationary process. The term, statistical homogeneity, is also used if the random variables are oriented in space.

Statistical inference is a statistical procedure in determining the appropriateness of a certain model to a specified problem by utilizing a limited amount of data and develops estimates of the essential parameters.

Statistically anisotropic is a term that relates to a random field in which its covariance function depends on both the magnitude and direction of the separation vector (i.e. the distance between two locations of random variables in the field).

Statistically isotropic is a term that relates to a random field in which its covariance function depends only on the magnitude of the separation vector. It does not depend on the direction of the separation vector.

Stochastic process is a term that refers to a process that contains a set of random variables. This process needs to have not only its probability distribution function but also a joint probability distribution between all points in space and time to characterize the process completely. Therefore, in the stochastic process, the terms auto- and cross-covariance are introduced to quantify the spatial and time correlations between random variables.

Stream flow-routing (or flood routing) is a procedure to determine the time and magnitude of flood wave at a point in a stream by utilizing the known data at one or more points upstream.

Transmissivity is the amount of fluid that can be transported through a porous medium per unit width per unit hydraulic gradient of the entire thickness of an aquifer. Its unit is (square of Length/Time). This concept is applicable only in two-dimensional flow. In the three-dimensional flow, this concept is meaningless.

Validation is the process to check whether a site-specific model performs similar to a real field system.

Variogram (γ_h) or semivariance: A variogram is "half the average of squared difference between the paired data values" (Isaaks and Srivastava, 1989).

$$\gamma(h) = E\{v(h)\} = \frac{1}{2}E\{(y(x+h) - y(x)^2)\} \qquad \text{(E6)}$$

and it can be estimated by

$$\gamma(h) = \frac{1}{2N_p}\sum_{i_p=1}^{N_p}\left[y(x+h) - y(x)\right]_{i_p}^2 \qquad \text{(E7)}$$

where

N = the number of data that are located separately with the lag (distance) of h

y = the measurement value of parameters

h = the lag or separated distance between data

v_j, v_i = the values of data at point j and I

i, j = the location of the measured data. The letter h indicates the distance between the measurement points j and i.

Note: for second-order stationary (i.e., $\sigma^2_{y_x} = \sigma^2_{y_{x+h}} = \sigma^2_y$) the following condition is true.

$$\gamma(h) = \sigma_y^2 - Cov_{yy'}(h) \tag{E8}$$

where σ_y^2 = the variance of y

Verification is the process to check whether a model solves the set of equations correctly same as the objectives of the equations.

APPENDIX F

RESIDUALS BETWEEN "TRUE" AND ESTIMATED VALUES OF HYDRAULIC CONDUCTIVITY AND MODFLOW PREDICTIONS

This appendix provides plots of residuals between the "true" and estimated values of hydraulic conductivity in the study domain. In addition, four forward analyses using MODFLOW are performed in order to determine the significance of using true or estimated hydraulic conductivity values. The hydraulic heads at the observation wells and the water balance in the aquifer, calculated by forward analyses using true and estimated hydraulic conductivity values, are discussed.

Residuals

In general, the residuals between the estimated and "true" values of hydraulic conductivity obtained in Case 1 of verification are relatively small while those obtained in Case 2 are large. The actual residuals and the ratio of residuals to the "true" values of hydraulic conductivity are presented in Figs. F1, F2, F3, and F4, respectively. The residuals mostly have positive values. It means that the estimated values of hydraulic conductivity, in general, are bigger than the "true" values of hydraulic conductivity". The maximum residual in Case 1 and Case 2 are about 13 m/d and 27 m/d respectively. The negative values appear in Fig. F1 and F4 must not be interpreted as negative values of hydraulic conductivity. The residuals at nodes around observation wells are, in general, smaller then the residuals at nodes located far away from the observation wells. However, at some nodes located close to the observation wells also have large values of residual. There are also many nodes that have zero residual even though these nodes located far from the observation wells.

The ratios determined by dividing the residuals with "true" values of hydraulic conductivity, are presented in Figs. F3 and F6. There is a large variation in these values. For example, the ratios vary between 0 and 0.5 in Case 1 and between 0 and 2.4 in Case 2. At nodes with large ratios, the actual residuals are not necessarily large. The value of ratio might be large because the "true" values of hydraulic conductivity at these nodes are small.

Figures F3 and F4 show the plot of residuals at nodes versus distance of those nodes to the closest observation well. The plot shows that the residual are, in general, also randomly distributed in the study domain. The residual are not always smaller at the nodes close to the observation wells compared to the nodes located far away from the observation wells.

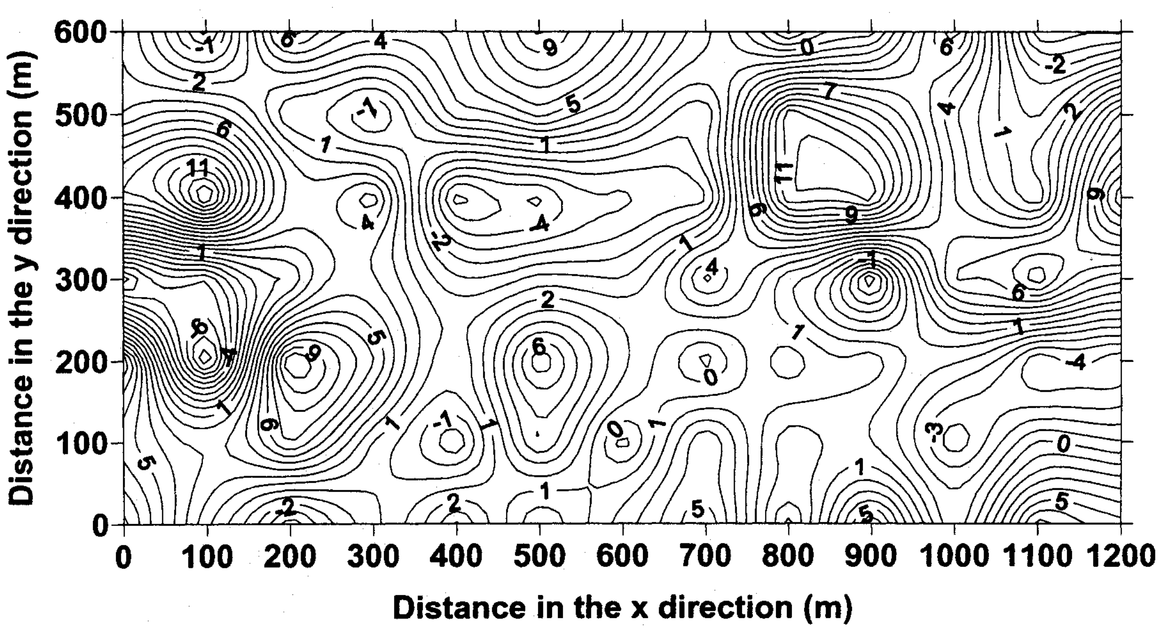


Figure F1 Residuals (m/d) between the "true" and observed hydraulic conductivity values at nodes – Verification Case 1

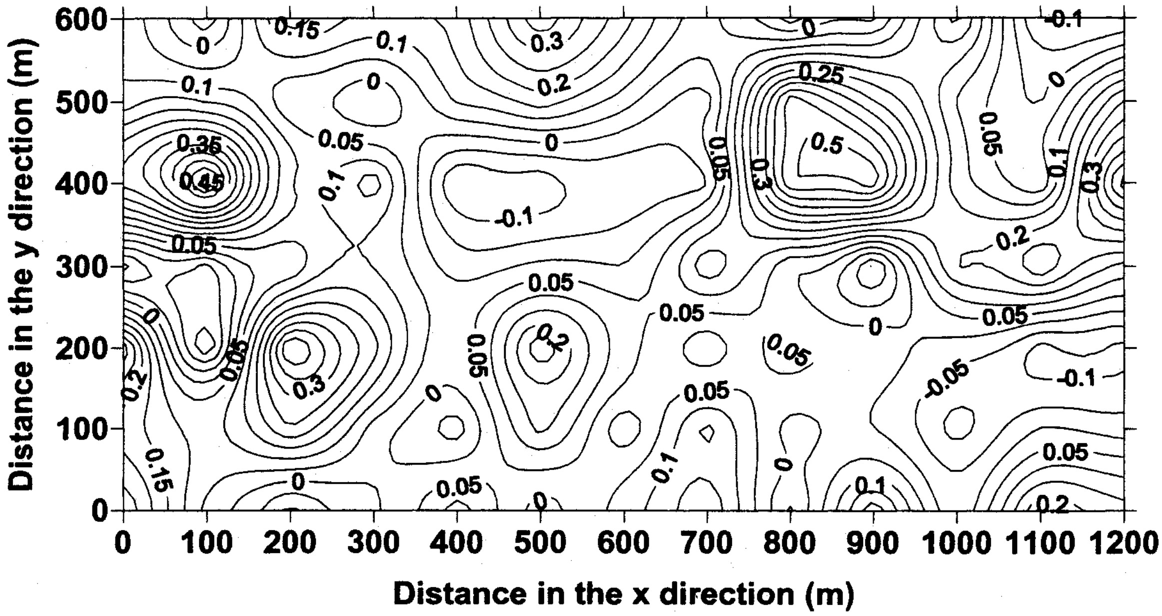


Figure F2 Ratio of residuals between the "true" and observed hydraulic conductivity values at nodes to the "true" values of hydraulic conductivity at the same nodes – Verification Case 1

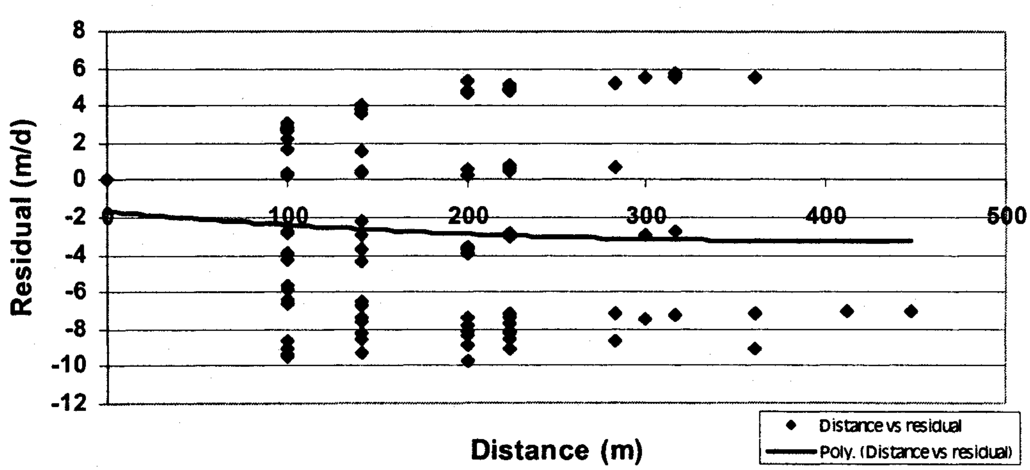


Figure F3 Distance of nodes from closest observation wells vs. residuals between the estimated values of hydraulic conductivity at those nodes and at the observation wells – Verification Case 1

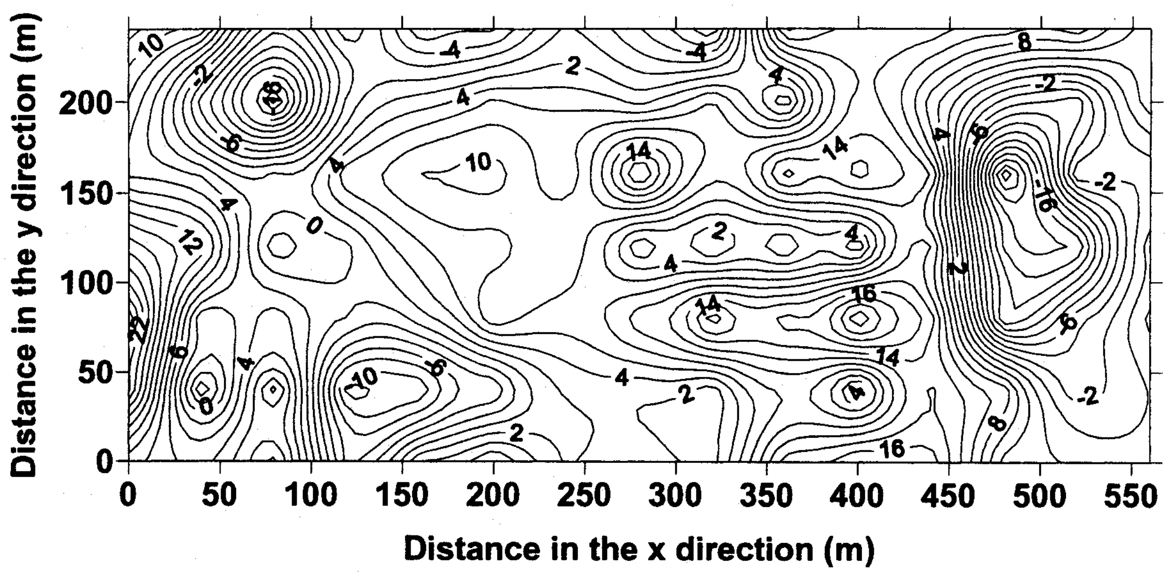


Figure F4 Residuals (m/d) between the "true" and observed hydraulic conductivity values at nodes – Verification Case 2

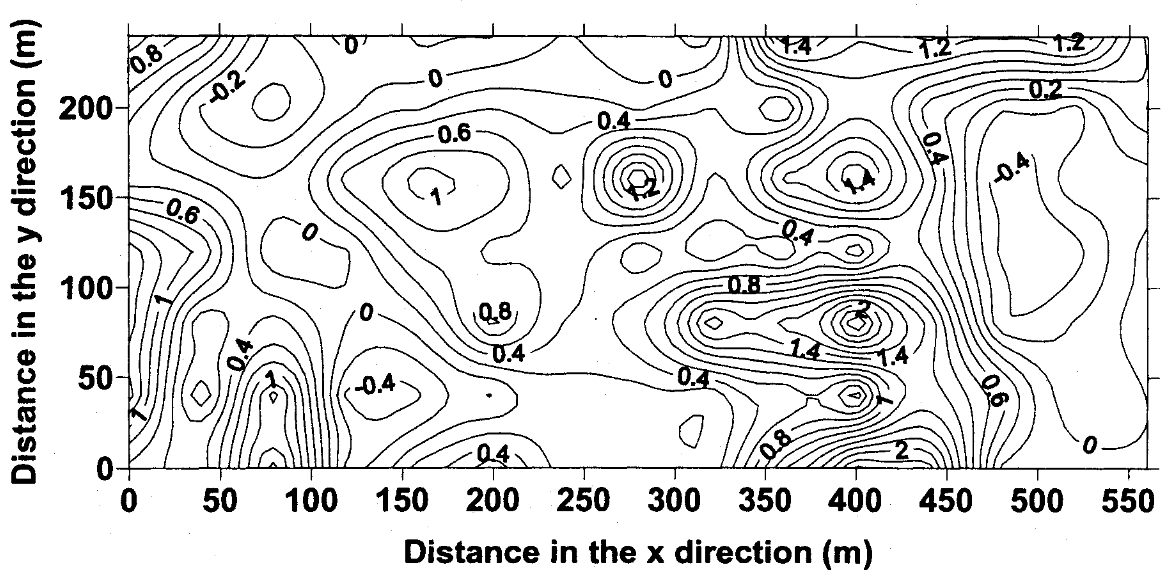


Figure F5 Ratio of residuals between the "true" and observed hydraulic conductivity values at nodes to the "true" values of hydraulic conductivity at the same nodes – Verification Case 2

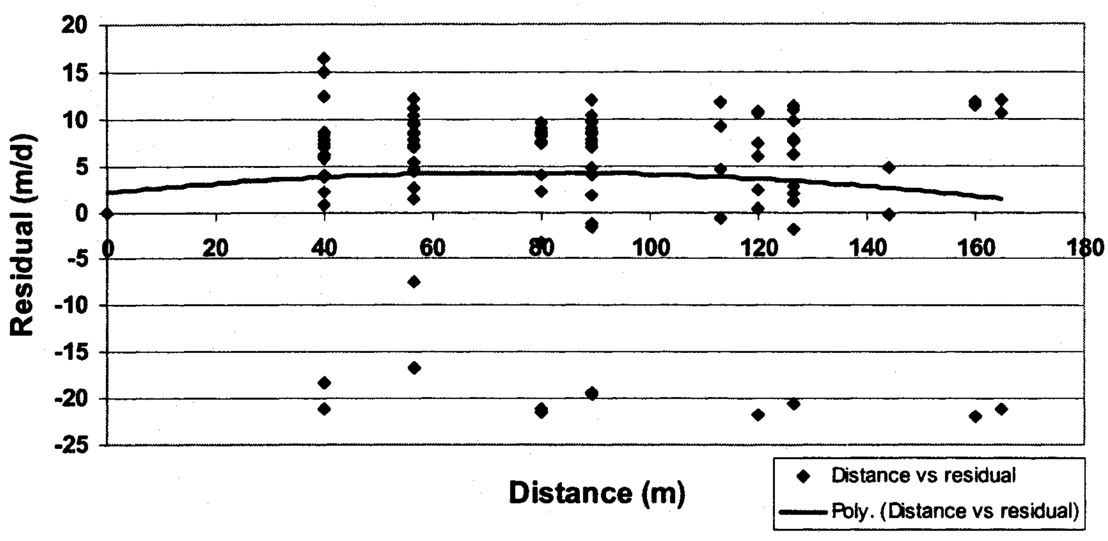


Figure F6 Distance of nodes from closest observation wells vs. residuals between the estimated values of hydraulic conductivity at those nodes and at the observation wells – Verification Case 2

Predictions

Predictions are made using MODFLOW. Forward analyses are performed for both steady state and transient flow in the aquifers used in Case 1 and Case 2 of the verification study. In the predictions, both the "true" and estimated values of hydraulic conductivity are provided as input.

In the steady state flow problem for Case 1, the discharge from the pumping well is assumed to be zero. The amount of discharge from the boundaries of the aquifer after 1 day is calculated first using the "true" values of hydraulic conductivity. Then, the estimated values of hydraulic conductivity are used as input in the analysis. The amount of discharge is 8333 m^3/d in the first analysis. In the second analysis, the calculated discharge is 8385 m^3/d. The difference is 52 m^3/d or about 0.6 %. These calculations are repeated for Case 2 of the verification study. When the "true" values of hydraulic conductivity are provided as input, the total amount of discharge at the boundaries of the aquifer is 2928 m^3/d. When the estimated values of hydraulic conductivity are used as input, the total amount of discharge becomes 3284 m^3/d. The difference between these discharge values is 356 m^3/d or about 12.2 %.

In the transient flow problems, there is a discharge of 4000 m^3/d at the pumping well. For Case 1 of the verification study, the use of true values of hydraulic conductivity results in the net amount water coming into the aquifer from the boundaries in 20 days is 71818 m^3. The amount of water lost from the storage is 8182 m^3. When the estimated values of hydraulic conductivity are used, the corresponding values become 72749 m^3 and 7251m^3.

For Case 2 of the verification study, the use of true values of hydraulic conductivity results in the net amount water coming into the aquifer from the boundaries in 50 days is 198625 m^3. The amount of water lost from the storage is 1375 m^3. When the estimated values of hydraulic conductivity are used, the corresponding values become 198464 m^3 and 1536m^3.

The difference between the results produced by using the true and estimated hydraulic conductivities can be expressed in percentage as follows. In Case 1, the difference is 1.3% for the net inflow from the boundaries and 11.4% for the amount of water taken out from the storage. For Case 2, the corresponding values of differences are 0.08% and 11.7%.

Figures F7 and F8 show that the predicted hydraulic heads (m) at observation wells obtained by using "true" and estimated values of hydraulic conductivity do not differ much. In Case 1, the maximum difference is about 15 cm, while in Case 2, the maximum difference is about 53 cm. These results show the use of the "true" and estimated values of hydraulic conductivity produce hydraulic head values very close to each other.

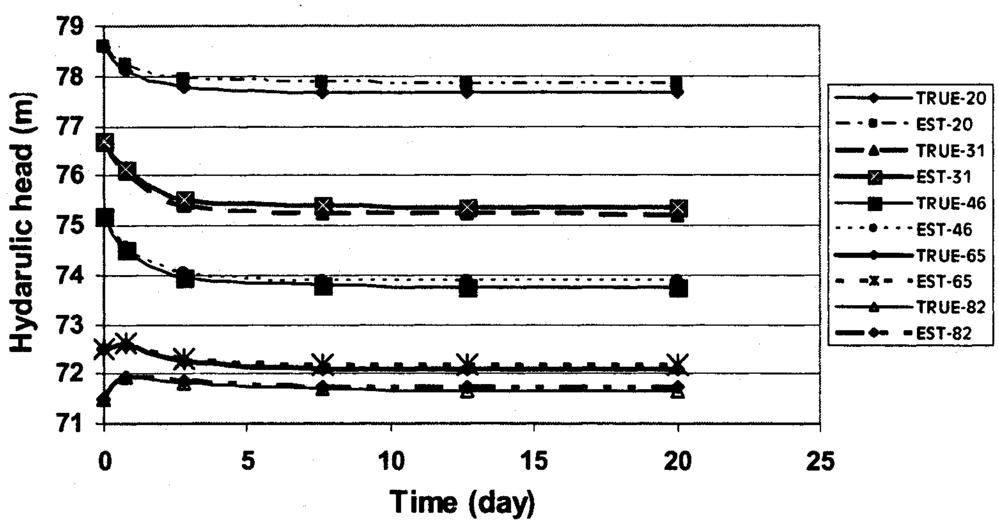


Figure F7 Comparison between predicted hydraulic heads (m) at observation wells obtained by using "true" and estimated values of hydraulic conductivity (Case 1)

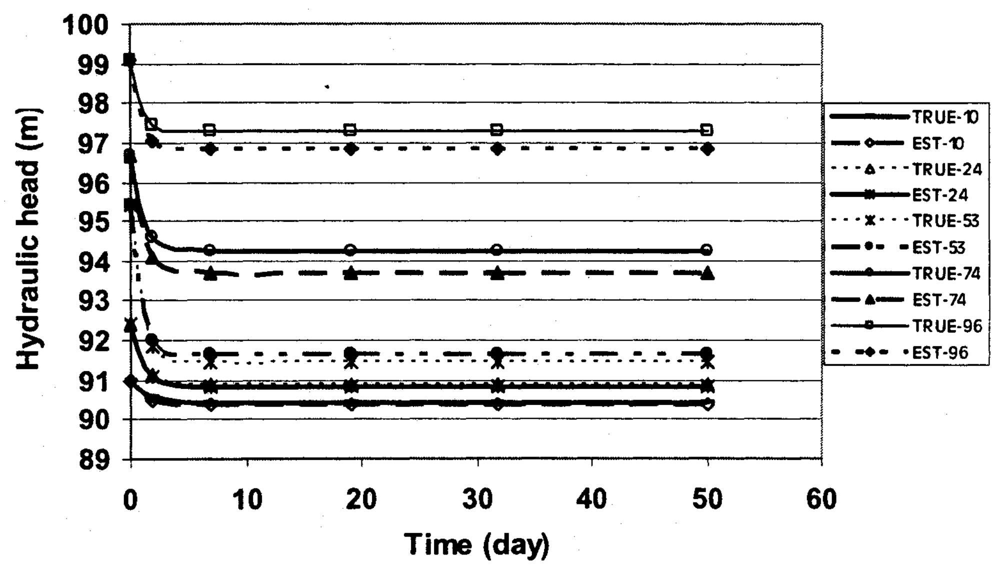


Figure F8 Comparison between predicted hydraulic heads (m) at observation wells obtained by using "true" and estimated values of hydraulic conductivity (Case 2)

The results presented in this appendix show that the estimated values of hydraulic conductivity can be used for the purpose of groundwater management in an aquifer.