A METHOD OF MODIFYING PARAMETER ZONATION TO OBTAIN A BETTER CONDITIONED GROUNDWATER INVERSE PROBLEM

by

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ABSTRACT

The purpose of this study is the determination of the transmissivity function of the groundwater flow equation under steady state flow conditions. A zonation approach for representing the transmissivity function is employed in the numerical model. The solution of the inverse problem follows the traditional indirect approach in which the sum of the squares of errors is minimized using Marquardt's minimization algorithm, penalty functions to impose linear constraints on the parameters, and the computation of the correction step length to help convergence to a feasible solution. The Marquardt method of minimization of the least squares function requires a direct solution for the heads for a given set of parameters. This direct solution for the heads is obtained using traditional finite element techniques. Errors from domain discretization and boundary condition representation are neglected in this study.

The problem of model overparameterization is handled by the elimination of ill-determined parameters during the minimization process. The covariance of the sensitivity matrix provides the information necessary to eliminate ill-defined parameters from the solution. The shape of the zones of a reduced parameter set model is determined by the selection of the zonation pattern which yields maximum sensitivity among models of reduced parameter dimensions. Model sensitivity is evaluated in terms of the determinant of the design matrix. Increased sensitivity in a model of reduced parameter dimensions can lead to a more stable solution. The effectiveness of the proposed algorithm is demonstrated by their application to a simple hypothetical one-dimensional aquifer with known analytical solutions for the

head and sensitivity coefficients (Appendix II) and the calibration of a steady-state model for a portion of the Floridan Aquifer in Jackson County, Florida using available scattered field data (Chapter 5). The results of the numerical experiments indicate that despite the difficulties inherited in the inverse problem due to model insensitivity and inadequate field data, it is possible to increase the reliability of the estimated parameters in such a way that a feasible solution can be obtained for field applications.

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LIST OF SYMBOLS

A	Sensitivity or design matrix
B	Second-derivative term matrix in Newton's method of minimization
b	Vector of estimated parameters
b_{LS}	Vector of least-squares estimated parameters
E	Squared error between observed and predicted head
F, f, Q	Vectors of sink/source terms
f_1, f_2	Boundary function of known terms
G	Parameterization matrix
g	Column vector used in the optimization of nonlinear functions
g_s	Scaled column vector in Marquardt's method
H	Hessian matrix
h	Hydraulic head
h_1, h_n	Head boundary function
I	Identity matrix
J	Jacobian matrix
K	Matrix of head differences
L	Lagrange function
n	Number of head data observations
P	Covariance matrix of the parameters
p	Number of parameters in the identification problem
r	Correlation coefficient
S	Scaled design matrix in Marquardt's method
Std. error	Standard error of identified parameters
s^2	variance of the residuals
T	Transmissivity
t	Time
U	Orthogonal matrix
U_T	Sensitivity coefficient with respect to transmissivity
V	Transpose of U
W	Diagonal matrix
X	Vector of spatial coordinates
x,y	Spatial coordinates

LIST OF SYMBOLS (Cont.)

$\wedge$	Indicates measured value
α	Parameter estimate correction factor
β	Vector of model parameters
ε	Error tolerance
Δh	Change in head produced by change in T
ΔT	Change in T
$\delta(x-x_o)$	Dirac delta function
δ_p	Vector of parameter corrections
Φ	Objective function
Γ	Boundary region
λ	Lagrange multiplier or eigenvalue of the sensitivity matrix
μ	Scalar to condition the design matrix in Marquardt's method
Ω	Groundwater flow domain
ρ	Acceleration parameter
Ψ	Equality constraint function used in the penalty function method
ψ	Finite element linear interpolation function
ζ	Penalty function
∇	Gradient operator

CHAPTER 1

INTRODUCTION

Groundwater resources are playing an increasingly important role in the general use and management of regional water resources world wide. The demand for groundwater for municipal, agricultural, and industrial use has steadily increased making this resource of vital importance to its users. Efficient management strategies for the resource require careful planning that can only be obtained with the use of mathematical models. Such management requires decision making concerning spatial distribution, rates, and timing of pumping in a region. The reliability of results obtained by mathematical models depends on the knowledge of model parameters used to account for the hydrogeologic features of the aquifer. Therefore, one of the most important problems in the application of such models is the evaluation from input-output data of those parameters which are not available from direct observations. This must be done to ensure that the model's response to given management policies will correspond in some "optimal" manner to the measured response of the aquifer itself. This problem is known as the inverse or parameter identification problem and a robust solution for field applications is yet to be found. As it will be discussed later in more depth, low-amplitude random errors in the piezometric head data along with inappropriate model representation of the parameter space, boundary conditions, and other modeling elements, tend to cause severe spatial oscillations in the solution process for the parameters.

Practical applications of numerical models as planning tools often fail because of the lack of appropriate field data which include aquifer properties which must enter the model as parameters. Direct field and laboratory measurement techniques such as

pumping tests and core analyses provide only scattered and inaccurate information about the spatial distribution of these parameters. The need for adequate aquifer parameter information has inspired scientists over the past three decades to develop aquifer parameter identification procedures which, as far as we know, have yet to give reliable results in groundwater management field applications.

This study is about the analysis of the groundwater inverse problem, particularly the development of an algorithm which makes the solution compatible with the quantity and quality of the head field data.

GROUNDWATER PARAMETER IDENTIFICATION

The successful application of groundwater models for management purposes depends upon the knowledge of several modeling elements such as natural recharge, transmissivity and storativity distributions; boundary conditions; interior and boundary recharge and discharges; and the ability of the numerical model to incorporate such information into the solution. Drilling wells and pumping tests are costly operations and are limited to a few locations within the time-space domain. For an inhomogeneous medium, the dimension of the parameter space is theoretically infinite. Therefore, for practical purposes, the parameter space is usually approximated by a finite-dimensional space.

In a deterministic frame the spatial distribution of T can be obtained by interpolating among the measured values but because of large and irregular variations in the T values, which usually prevail in aquifers, such procedure is bound to fail, by leading to unrealistic values. On the other hand, head measurements are usually more abundant, since installation of piezometers and reading of water levels are simpler and cheaper operations than pumping tests. The usage of these measurements in order to improve the quantitative characterization of the transmissivity spatial

distribution, as well as the other poorly known parameters (natural recharge and boundary conditions) is known in the literature as the inverse problem.

Analytical solutions based on curve matching techniques are limited to a single well or a well field. For larger scale problems where an entire aquifer is under investigation, trial and error techniques are usually employed. With the aid of numerical techniques, a set of parameters is subjectively adjusted until the computed head distribution closely resembles the observed head data. This procedure is time consuming and is impaired by the problem of nonuniqueness of the solution. These difficulties associated with the trial and error procedure along with the development of high speed computers over the last three decades, have led to a great number of new techniques to approach the inverse problem solution. Direct approach solutions can produce fast and efficient solutions if abundant and relatively accurate head and boundary conditions data are available.

A more popular solution approach, the indirect approach, has found more acceptance because of the less data required to yield a solution. This technique is designed to approach the optimum estimates of the parameters in a systematic way while minimizing an error norm related to the observed and simulated heads.

Despite their ease of application, indirect techniques can be plagued with problems such as instability and nonuniqueness of the solution. Not until recently has the determination of the optimum dimension of the parameter space, relative to the amount and quality of head data, been incorporated as an integral part of the identification problem to control instability and improve uniqueness of the solution.

SCOPE AND CONTENTS OF THE STUDY

The primary objectives of this study are: (1) to gain insights into the development of numerical and theoretical techniques for the improvement of current

mathematical identification models; (2) to apply and verify the technique's applicability using real field data.

The type of system chosen for identification can be described as an inhomogeneous, isotropic aquifer under confined steady state conditions. It can be pointed out that the algorithms developed in this study can be applied in the same manner to a transient problem assuming that the storativity distribution is known. Steady state parameter identification usually finds more difficulties than the transient case because the head data available only provides information for one stress scenario. Therefore, the inverse methodologies developed for steady state conditions will be more robust that if they are developed for a transient case.

The mathematical representation of the steady state inverse problem is given by a linear partial differential equation of parabolic type with respect to the hydraulic head. The determination of the T distribution in this equation depends on the head data available at scattered locations throughout the aquifer. Lack of informative head data and the errors in the measured heads lead to instability and nonuniqueness of the solution. In this study, the possibility of improving the accuracy and reliability of the estimated transmissivities is investigated through the adjustment of the dimension of the parameter space relative to the amount and quality of the observed head data.

Before presenting the development of the identification algorithms, it is necessary to review the state-of-the-art about groundwater parameter identification. Chapter 2 presents a brief review of previous studies on different areas of parameter identification. Most methods discussed herein fall within three categories: direct, optimization, and statistical methods. It is also suggested that the optimization approach is more reliable and applicable for the identification of transmissivities.

Chapter 3 presents the formal mathematical representation of the identification problem in terms of the optimization approach. The Marquardt method for the

solution of the nonlinear least squares problem is presented as the method of solution. Mathematical artifacts such as matrix scaling, step size determination, and incorporation of prior information in the form of linear inequality constraints are revised and incorporated into the Marquardt algorithm in order to improve its convergence properties.

In Chapter 4, the groundwater parameter identification problem for a confined aquifer under steady state conditions is formulated in terms of least squares optimization and then solved with the algorithms proposed in Chapter 3. Special attention is paid to the control of the dimension and the variations in the parameter space required for a well-posed and stable solution. This control of the dimension of the parameter space is called parameterization and is achieved with the aid of statistical measures related to the reliability of the estimated parameters. In this chapter, the finite element method is used to solve for the heads and its derivatives over the discretized aquifer. The computed head distribution is required in the optimization algorithm to update the value of the objective function, whereas the derivatives are used to compute the corrections applied to the estimates.

Chapter 5 illustrates the application and performance of the proposed identification algorithms to a steady state confined aquifer in Jackson County, Florida, with hypothetical and noisy field data. Also, Appendix II describes in detail the application and verification of the numerical techniques used in the forward solution for the heads and sensitivity coefficients and the identification of the transmissivities in a one-dimensional aquifer with a known analytical solution. Special attention is given in this appendix to the parameter zonation procedures of Chapter 4 to improve the convergence properties of the minimization algorithm.

Finally, a brief summary of the development and application of the proposed techniques is presented, along with the conclusions in Chapter 6.

CHAPTER 2

REVIEW OF PREVIOUS RESEARCH

Aquifer parameters are usually determined based on graphical curve-matching techniques under the assumptions that the aquifer is homogeneous and isotropic and a closed-form solution for the governing equation exists. These methods provide only an areal average value of transmissivity and storage coefficient and, therefore, cannot be applied in situations where the above model assumptions do not apply.

Model calibration by trial and error methods is a technique that can only be applied in the simplest cases. Adjustments to the parameter set during the calibration process are made based mainly on the criterion and experience of the modeler. Uniqueness of the solution cannot be guaranteed even with a set of parameters that closely reproduces the observed hydraulic head distribution.

DIRECT AND INDIRECT APPROACH

Most published methods on the groundwater inverse problem fit into the classification established by Neuman [1973]: "Direct" and "Indirect" methods. In the direct approach, the parameters, usually transmissivities and/or storativities, are treated as independent variables in a formal boundary value problem. The head variations and derivatives, usually numerically estimated, are assumed known over the entire flow region. The parameter distribution is approximated by continuous functions of the spatial coordinates. It is also fundamental in this method that each parameter be associated with one non-zero coefficient $\partial h/\partial x$ at each point of the region, otherwise, a unique solution cannot be guaranteed. Given these requirements, the solution of the problem is equivalent to that of a linear first-order hyperbolic partial differential equation. The errors induced by interpolating for the head values

along with the observation errors, result in an error when solving for the dependent variables. This error is then minimized over the proper choice of the parameters. The following are some of the most relevant papers related to the direct approach: Nelson [1968], Kleinecke [1971], Emsellem and de Marsily [1971], Neuman [1973], Frind and Pinder [1973], Nutbrown [1975], Sagar et al. [1975], Yakowitz and Noren [1976], Navarro [1977], Britles and Morel [1979], Ponzini and Lozej [1982] and Yeh et al. [1983].

The indirect approach to the solution of the inverse problem has also been the subject of intense research over the past two decades. This approach is a trial and error procedure that seeks to improve an initial set of parameter estimates in an iterative manner until the model response has satisfied an error criterion. The main advantage of this method is that the formulation of the inverse problem is applicable to situations where the number of observations is limited and does not require the interpolation or approximation of the hydraulic head on the entire flow region. A disadvantage of this approach is that minimization is usually nonlinear and nonconvex leading to instability and nonuniqueness during the numerical solution. Among the most relevant research in this area of the groundwater inverse problem we can mention the research of Jacquard and Jain [1965], Jahns [1966] Thomas et al. [1972], Coats et al. [1970], Cooley and Sinclair [1976], Haimes et al. [1970], Yeh [1975,b], Chang and Yeh [1976], Hefez, et al. [1975], Bellman and Kalaba [1965], Yeh and Tauxe [1971a,b,c], Marino and Yeh [1973], Vemuri and Karplus [1969], Chen et al. [1974], Chavent et al. [1975], Yoon and Yeh [1976], Cooley [1977], Bruch et al. [1974], Khan [1986], Garay et al. [1976], Distefano and Rath [1975], Sadeghipour and Yeh [1984], Yeh and Sun [1984] and Lu et al. [1988].

Most of the previous research about direct and indirect methods to the inverse problem are presented in the paper by Yeh [1986]. This paper represents a

comprehensive review of direct and indirect approaches to the solution of the inverse problem.

BAYESIAN ESTIMATION

In more recent years, Maximum Likelihood (ML) techniques derived form the application of the indirect approach and statistical techniques have been applied with some success to the groundwater inverse problem. In general, these methods require prior information and therefore are also known as Bayesian methods. ML methods consider the model parameters as deterministic quantities subject to uncertainty because of inadequate prior information. The inclusion of prior hydrogeologic information into the inverse problem can significantly reduce the ill-conditioning of the problem and the statistical uncertainty of the estimated parameters. The information from prior data reflected by the likelihood function is combined with the prior density function of the parameters to define the posterior density function. The estimates are obtained using this new density function.

Parameters obtained by Bayesian methods are biased estimates because of the weight given by the prior distribution to the parameters with higher probabilities. One way of reducing the bias effect is to provide sufficient sample data to overweight the effect of the prior distribution.

Gavalas et al. [1976] used this approach instead of the parameter zonation to reduce the uncertainty of the permeability estimates in a simulated one-dimensional oil reservoir. They found that the results from the bayesian estimation were more accurate than the zonation. This method also showed improved convergence of the iterative Gauss-Newton minimization algorithm.

Expanding on the work of Gavalas [1976], Neuman and Yakowits [1979] developed a technique that involves the solution of a family of generalized nonlinear

regression problems and then selecting one particular solution from this family by a comparative analysis of residuals. Prior information about the transmissivities was incorporated directly into the solution process by an extended Bayesian regression approach in which the prior information vector is related to the real transmissivity vector via an additive noise vector with known statistical characteristics. Numerical experiments on hypothetical aquifers showed the effectiveness of this method. Further refinements of this method were later reported by Neuman [1980]. This improved method was based on an efficient variational method developed by Chavent [1971] for computing the sensitivity coefficients. Finite elements with linear basis functions were used as the basis for the solution of the groundwater flow equation. The inverse problem was posed in terms of log transmissivities instead of transmissivities. It was then solved by a Fletcher-Reeves conjugate gradient algorithm in conjunction with Newton's method for determining the step size at each iteration. Results from two theoretical examples showed that this method may be capable of computing log transmissivity estimates with an error variance much smaller than that of the original (or prior) log transmissivity data.

Carrera and Neuman [1986a,b] developed a different maximum likelihood solution technique extended to induce penalty criteria based on prior information on the parameters. In this study it was assumed that not all the factors that contribute to the prior errors can be quantified statistically at the outset. The covariance matrices of these errors were expressed in terms of several parameters that, if unknown, can be estimated jointly with the hydrogeologic parameters by a stepwise optimization process. The estimated parameters included values and directions of principal hydraulic conductivities (or transmissivities) in anisotropic media, specific storage, interior and boundary recharge or leakage rates, coefficients of head-dependent

interior and boundary sources, and boundary heads. Application to synthetic and field data of this method was reported by Carrera and Neuman [1986c].

Kalman filtering is another Bayesian method that has been used in a variety of inverse problem studies. This method was originally developed in the field of optimal control [Kalman, 1960] and requires expressing the groundwater model in terms of the state-space formulation that consists of a vector state equation and a vector observation equation. The state vector is augmented to include the parameter vector as another state variable. Assuming that the errors have zero mean and are of white Gaussian process with known covariance matrices, Kalman filtering can then be applied for simultaneous recursive state and parameter estimation. The work by Wilson et al. [1978] used an extended Kalman filter accounting for model and measurement error. The prior information includes information about the parameters, information taken from input-output measurements to improve the estimates, and the system state.

STATISTICAL APPROACH

The statistical approach is a different approach to the identification problem that has emerged in the last few years from ideas of the Bayesian approach. This method does not attempt to determine the precise values of the parameters or their space averages as is the case in the deterministic methods. Instead, it seeks to employ data and the equations of flow in order to estimate the expected values of the parameters and their variance or some related measure of their error. The work by Kitanidis and Vomvoris [1983] demonstrated the applicability of the statistical method in a one-dimensional case using synthetic data. Subsequently the method was expanded and applied to two-dimensional steady state synthetic flow data by Hoeksema and Kitanidis [1984] to estimate the unknown transmissivity field. An

application to synthetic steady state flow was presented by Dagan [1985]. Other studies related to geostatistical methods are the studies by Delfiner and Delhomme [1973], Delhomme [1979], and de Marsily [1982].

ILL-POSEDNESS CHARACTERISTICS OF THE INVERSE PROBLEM

The importance of parameter identification in connection with groundwater resource management has been well established. However, the application of parameter estimation has not been completely resolved mainly because of the limitations of current techniques to deal with the ill-posedness of the problem. Nonuniqueness, instability, and nonidentifiability have been pointed out by hydrologists as the result of the ill-posedness and the reasons the inverse problem in most practical situations cannot be satisfactorily solved. However, it has not been clearly established what the rule of each of these conditions is and under what circumstances a meaningful solution is possible.

Uniqueness

Nonuniqueness in the inverse problem is an inherent condition that arises whenever the number of distributed parameter types to be identified exceeds the available number of independent sets of equations or data. When solving the inverse problem, the parameter space $T(X_i)$, where T is a continuous function of the spatial coordinates vector, X_i, is discretized so that the solution can be obtained at a finite number of points. For illustration, let us consider the steady state, anisotropic aquifer case whose partial differential equation governing the flow potential is:

$$\nabla (T \nabla h) - f = 0 \qquad (2.1)$$

subject to the following boundary conditions:

$$h(X_i) = h_1(X_i),\ X_i \in \partial\Omega_1 \tag{2.2}$$

$$(T \nabla h)n_i = h_n(X_i),\ X_i \in \partial\Omega_2 \tag{2.3}$$

in which:

∇	=	gradient operator
X_i	=	spatial coordinates
h	=	flow potential in the aquifer
h_1, h_n	=	specified function of X_i
f	=	source or sink function
Ω	=	flow region
$\partial\Omega$	=	Boundary of the aquifer ($\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$)
T	=	transmissivity
n	=	normal direction

Equations (2.1) and (2.2) define a Dirichlet problem, whereas equations (2.1) and (2.3) define a Neumann type problem, and the combination of (2.1), (2.2), and (2.3) is known as a mixed boundary value problem. The application of a numerical method to solve the problem, as specified above, would lead to a system of algebraic equations such as:

$$\frac{\partial}{\partial X_i}\left(T_{ij}\,\frac{\partial h}{\partial X_i}\right) - f = 0 \tag{2.4}$$

subject to:

$$h(X_i) = h_1(X_i),\ X_i \in \partial\Omega_1 \tag{2.5}$$

and

$$T_{ij} \frac{\partial h}{\partial X_j} n_i = h_n (X_j), X_j \in \partial\Omega_2 \qquad (2.6)$$

In matrix form, equation (2.4) can be written as follows:

$$[K]_{NxNp} \{T\}_{Np} - \{F\}_{Np} = 0 \qquad (2.7)$$

where:

N = number of nodes
N_p = number of transmissivities
K = matrix of head differences between neighboring head values
T = vector of unknown transmissivities
F = vector of known source/sink terms

The solution of the inverse problem requires that the elements of matrix K be known along with the prescribed source/sink terms in F. Thus, the dependent variables contained in T are the unknown transmissivities for which we solve the system of equations in (2.7). Clearly the rank of the matrix K must be equal to N_p, the number of parameters for (2.7) to have a unique solution. Since K depends on the head gradient between neighboring nodes, they must be nonzero at least at one point in each element or zone for K to have the required rank. A measurement taken at one point where there is no sensitivity to a parameter which is to be identified, would cause this rank deficiency problem. For the particular case where no internal source/sink terms are specified and all the boundary conditions are of the no-flow or prescribed head type, (2.7) becomes:

$$K\ T = 0 \qquad (2.8)$$

Here, rank K < N_{p-1} < N_p, therefore, the problem has no unique solution as multiplying K by a constant has no effect on the computed heads.

In practical applications of the inverse problem, it is common to find areas of zero or near-zero $\partial h/\partial X_i$. Therefore, it is important to understand the conditions under which the system is not identifiable in connection to information from observation wells, boundary conditions and pumping wells. Chavent [1975] presented a detailed study of the uniqueness problem in connection to parameter identification in distributed systems.

Identifiability

Parameter identifiability is generally related to the quality and quantity of information to distinguish between alternative set of parameters. This lack of information usually translates into unidentifiable parameters simply because the data is not sensitive to the values of the parameters over certain areas of the aquifer. This may lead to a nonunique solution of the problem. To investigate this condition, scientists have developed identifiability conditions, applicable for certain classes of inverse solutions. These identifiability conditions define the conditions under which a set of parameters can be uniquely estimated. The application of identifiability conditions prior to the solution of the inverse problem can provide insight to avoid the problem of nonidentifiable parameters, or, as in the case of least squares estimation, slow convergence or nonconvergence towards a local minimum.

For linear or nonlinear least squares estimation, Beck and Arnold [1977, p. 481] define an identifiability criterion that applies equally to least squares, weighted least squares, and maximum likelihood estimation with normal errors. This condition implies that the (continuous) sensitivity coefficients must be linearly independent over the range of measurements for all the parameters to be uniquely and

simultaneously estimated. This condition is usually true only when a small number of parameters are being identified.

Kitamura and Nakagiri [1977] studied the identifiability of a linear, one-dimensional parabolic partial differential equation. They defined identifiability as the conditions under which an "identifiable" parameter can be determined uniquely in all points of its domain by using the input-output relation of the system and the input-output data.

If different sets of parameters lead to a given head distribution, the parameters are not identifiable. In practical applications, the parameters are obtained from sets of field data limited in quality and quantity and therefore compromising the identifiability of the parameters. Some of the identifiability problems have been resolved by reducing the dimensionality of the parameter space. Two methods have been used to reduce the dimensionality of the parameter space: (1) zonation, in which the flow region is divided into a number of subregions, or zones, and a constant parameter value is used to characterize each zone. The transmissivity function is then represented by a number of constants which equal to the number of parameter zones; and (2) interpolation functions, which is the classical application of finite elements where the flow region is divided into several elements connected by nodes. Each node is associated with a local basis function. The transmissivity function is now represented by a linear combination of the basis functions, and the parameter dimension is the number of unknown nodal transmissivity values.

Several studies on parameterization using zonation have been published in the literature, among them Jahns [1966], Coats et al. [1970], Thomas et al. [1972], Yeh and Yoon [1976], Cooley [1977] and Neuman and Yakowitz [1979]. The interpolation method has been used by Frind and Pinder [1973], Distefano and Rath [1975], Yoon and Yeh [1976], and Yeh and Yoon [1981]. Instead of using linear

combinations of basis functions, Sagar et al. [1975] used a spline interpolation scheme. Authors of examples of geostatistical methods applied to parameterization that can be found in the literature are: Yeh et al. [1983], de Marsily [1982], Kitanidis and Vomvoris [1983] and Hoeksema and Kitanidis [1984].

Since field data cannot be made available at every computational grid node associated with the numerical solution of the groundwater equation, identifiability must be relaxed by an extended identifiability criterion which leads to a weak unique solution. Yeh and Sun [1984] established an extended identifiability criterion known as "δ identifiability." This criterion was used to design an optimal pumping test to assist parameter estimation. Also, Chavent [1983] presented a weaker identifiability criterion for output least square identification.

Stability

It is generally understood that the instability condition of the inverse problem is caused in part by noise in the head data and the errors associated with the optimization approach chosen for the solution. Its effect is observed by oscillations of the estimated parameters and premature termination of the search due to existence of local minima. Since error in the observed data is a source of instability, it is important to understand its origins and to develop techniques to minimize it in the field and during the numerical solution of the inverse problem. For practical purposes it is assumed that there are so many sources of error in field measurements that errors can be considered random. If an apparent bias is detected during analysis, it should be eliminated by analysis of model results.

Instability due to errors produced by model representation is inherent of the inverse problem regardless of the method of solution chosen. The hyperbolic partial differential equation governing the inverse problem does not have the smoothing

effect on the errors that the integration process provides in the forward solution when solving the second order elliptic or parabolic partial differential equation.

Some methods have been used in the solution of the inverse problem specifically aimed to control instability. Constrained optimization algorithms have been used in an attempt to limit the range of variation of the parameter estimates during the solution process. Among inverse solution algorithms that use this technique, are the work by Thomas et al. [1972] the box-type constraints, Sadeghipour and Yeh [1984], Yoon and Yeh [1976], Yeh and Yoon [1976], and Yeh and Yoon [1981], the Rosen's gradient projection constraints; and Distefano and Rath [1975], structure constraints. The use of the log transmissivities, Neuman and Yakowitz [1979], Neuman [1980], also provides a form of constraints on the parameters assuring positive values of the estimates. This method also reduces variability of the parameter space, and, as a consequence, improves the stability of the solution.

When the inverse problem is being solved by least squares minimization techniques, scaling of the sensitivity matrix have been reported to improve stability. This matrix scaling reduces variability among the elements of the least squares matrix. The use of this technique has been documented by Cooley [1977], Draper and Smith [1966, pp. 147-149].

Other methods used to control instability are ridge regression, Cooley [1977, 1982]; penalty function, Neuman [1973]; inclusion of prior information, Neuman and Yakowitz [1979], Gavalas et al. [1976], Neuman [1980], Cooley [1982], Carrera and Neuman [1976a]; and parameterization or reduction of parameter space dimension, Yeh et al. [1983], Emsellem and de Marsily [1971], Yeh [1976], and Shah and Seinfeld [1978].

In a recent study, Tucciarelly [1991], a new formulation is proposed to identify zoned transmissivities in confined aquifers. The new feature in this formulation is the weighting factors of the residuals used in the minimization of the norm. These weighting factors were the square of the estimated transmissivities. It was shown, by theoretical analysis and numerical experimentation, that this method can lead to improved global convergence properties and characteristics of stability in theoretical and practical field problems.

MODEL PARAMETERIZATION AND STRUCTURE IDENTIFICATION

For most practical problems, the amount and quality of field data is rarely adequate for identification purposes. There are usually more parameters than the number of observations sensitive to all the parameters. This lack of information, in terms of the number of parameters, is called model overparameterization and its effect is seen in ill-conditioned coefficient matrices obtained from the numerical integration of the groundwater flow equation. The application of parameterization methods is based on the fact that as the number of parameters decrease, the modeling errors will consequently increase but errors in the data will be more seriously reflected in the parameters. An optimum level of parameterization can be found which minimizes both the uncertainty in the estimated parameters and the error from the numerical discretization of the parameter space.

Traditionally, parameterization has been used in two different approaches: (1) the interpolation and (2) the zonation approach. The interpolation method of parameterization allows the parameter space to be a continuous function of the spatial coordinates. In this case, the parameter space is represented by a finite series of piecewise polynomials such as splines or finite element interpolation functions. In the other hand, the zonation method is in principle simple and easier to apply than the

interpolation method. In the zonation method, the aquifer is subdivided into subregions in which the parameter is assumed to have a constant value. Reduction of the dimension of the parameter space for parameterization by zonation is performed by simply combining a parameter with a neighboring one based mainly on prior geologic information. It has been determined from previous studies that the zonation approach yields as reliable head distributions as some interpolation methods [Yakowitz and Duckstein, 1980].

The zonation approach as applied in previous studies, [Yeh, 1976; Cooley, 1977; Neuman, 1980] leave the discretization of the parameter space to the judgment of the modeler. Hydrogeologic prior information can be used to discretize the parameter space but the problem of determining an adequate number of parameter zones is difficult to solve Too many zones and to few head measurements will inevitably lead to an unidentifiable case. To solve this problem, Gavalas et al. [1976] proposed a method of parameterization in which the estimate error of zonation has two components. One is due to the error of parameterization and decreases with an increasing number of zones. The other is due to statistical scatter and increases as the number of zones increases. The sum of the two errors attains its minimum at an intermediate number of zones. In this study Gavalas et al. discretized the parameter space of permeability (k) and porosity (ϕ) of a hypothetical one-dimensional aquifer into 33 equally sized intervals. The number of parameters was sequentially reduced by zoning the parameter space into smaller number of constant value segments (16, 8, and 4 zones). The errors in the obtained heads, J_ϕ , were calculated as well as the error in the parameters, J_k and J_ϕ. The error criterion J was the sum of squared errors. They observed that the minimum value of $J = J_p + J_k + J_\phi$ was attained at a number of zones between the 8-zone and the 16-zone case.

Expanding the work of Gavalas, et al. [1976], Shah and Seinfeld [1978] studied two cases of parameterization: (1) simple zonation, in which the parameter vector was a linear combination of some suitable set of orthonormal vectors and (2) zonation by sensitivity coefficients (the parameters were assumed to be a linear combination of the eigenvectors of the sensitivity matrix). The trace of the estimated covariance matrix was used as a measure of the estimate error. The example used to illustrate this technique is similar to the hypothetical case presented by Gavalas et al. [1976]. The objective of this study was to identify the optimum number of zones at which the sum of observation error plus parameterization (error given by the trace of the estimate covariance matrix) attains a minimum. The same conclusion was obtained for both cases of zonation techniques employed: the total error given by the trace of the covariance matrix, used as a measure of total uncertainty, reaches a minimum at a particular level of parameterization (at a particular number of zones). Concerning the type of parameterization, they concluded that the zonation is preferable when the location of the zone boundaries is suggested by geological information, otherwise, parameterization by sensitivity vectors provides somewhat better estimates. If prior information on the parameters is available, they recommended the use of a Bayesian estimation method which yielded more accurate estimates.

In a similar study by Yeh and Yoon [1981], finite elements were used to represent the unknown transmissivity function parametrically in terms of nodal values over a suitable discretization of a flow region. A modified Gauss-Newton algorithm was used for parameter optimization and covariance analysis to estimate the reliability of the estimated parameters. They noted that as the dimension of the unknown parameter increases, the modeling error represented by a least squares criterion will

generally decrease, but errors in data would be propagated to a greater degree into the estimated parameters, thus reducing the reliability of the estimated parameters.

In an effort to eliminate from the solution only ill-defined parameters, Yeh [1976] developed a zonation method of parameterization. In this method, the aquifer domain is subdivided into piecewise homogeneous subregions. Each subregion was characterized by a single parameter. The covariance matrix of the unknown parameters provided the parameter variances to identify ill-determined parameters. Then, parameter zones associated with well-determined parameters were subdivided into smaller subregions whereas zones associated with ill-defined parameters were combined with neighboring zones associated with well-determined parameters. The effectiveness of this method was demonstrated on a hypothetical two-dimensional, transient case.

Other authors who have used parameterization by zonation, perform the dimensionality reduction by combining adjacent parameter zones arbitrarily until a "best" pattern has been found [Jahns, 1966; Yakowitz and Duckstein, 1980; Carrera and Neuman, 1986c]. The optimal determination of the shape of zones in the zonation case, or the optimal determination of the location of nodes (nodal transmissivities) in the interpolation case, is called parameter structure identification. As pointed out by Sun and Yeh [1985], the determination of the parameter structure should be an integral part of the parameter estimation process. In this study, they presented an optimization method to identify parameter structure and the parameter values. The problem of identifying the parameter structure was formulated as a problem of combinatorial optimization. The parameterization technique consisted on identifying a structure matrix which can be used to represent a variety of parameter variations ranging from zonation to continuous distribution. Ignoring the errors resulting from the finite element discretization and using the covariance matrix

criterion [Yeh and Yoon, 1981] to evaluate the reliability of the estimates, they identified the parameter values, the optimal number of parameters, and the optimal parameter structure for three hypothetical examples.

In a recent study Keidser and Rosebjerg [1991] compared the performance of four different transmissivity characterizing methods to solve the groundawater inverse problem for flow and transport parameters (dispersion coefficients and dispersivities). Head and concentration data were used to identify the parameters in a two-stage approach. In the first stage the transmissivities were estimated using both the head and concentration data. Using this transmissivity field, transport parameters were identified in the second stage on the basis of the concentration parameters. Finally, the stage one estimation was repeated to adjust the transmissivities using the optimized transport parameters. Four methods were used to characterize the spatially variable transmissivities. The basic difference among the models was in the way prior information of transmissivity is incorporated into the model. The first three models reproduced point observations of transmissivity by means of the geostatistical method of kriging. Model one supplied the observations with estimated transmissivity values, model two adjusted the kriging estimates by means of correcting terms, model three adjusted the kriging model by optimizing the geostatistics of the transmissivity, and model four, pure parameter zonation, only used the inherent information to develop the zonation pattern. The authors concluded that the pure zonation approach, despite its simplicity, is generally superior to the data-dependent approaches in cases of limited data availability and poor data quality.

SUMMARY AND CONCLUSIONS

Three different approaches of solution to the inverse problem were identified in the literature. The direct approach can provide an efficient and fast solution to the

inverse problem. However, for most practical problems, errors induced by the interpolation of the head distribution and its derivatives along with measurement errors will inevitably deteriorate the solution. Existence and uniqueness of the solution cannot be guaranteed because of the lack of field information in the form of transmissivity values for the evaluation of boundary conditions and the presence of areas in the aquifer with zero or near-zero hydraulic gradient.

The indirect approach has found more acceptability because it deals more efficiently with data inadequacies by minimizing the total errors in a least squares fashion. It does not require interpolation for the heads and its derivatives and the boundary conditions for the parabolic-type equation are easier to satisfy in the form of boundary flows and constant head values. The solution by the optimization approach is carried out in an iterative manner, minimizing an error norm such as least squares. Severe ill-conditioning due to lack of accurate field measurements can make the solution process slow and unreliable. A number of numerical techniques to deal with the ill-conditioning of the inverse problem have been reported in the literature. Among the most useful numerical artifacts to control instability and nonuniqueness are the inclusion of prior information on the parameters by penalty methods or gradient projection techniques, scaling of the sensitivity matrix, step size control, and reduction of the parameter space dimension.

Finally, the statistical approach, a new technique with roots in Bayesian estimation, has demonstrated some promising results in models with synthetic data. Further development and testing will be required to successfully apply this approach to field problems with inadequate data.

CHAPTER 3

OPTIMIZATION METHODS FOR PARAMETER IDENTIFICATION

This chapter presents a brief overview of the formulation of the identification problem in terms of optimization procedures and their application to nonlinear parameter estimation. A brief discussion is presented on each of the elements involved in the optimization and their suitability and applicability to the solution of the groundwater parameter identification problem. Generally speaking, the solution of the identification problem by optimization techniques is based in the minimization of an objective function in terms of the parameters. In optimization problems it is critical, for an efficient minimization, to select the appropriate type of objective function. The use of constraints in the parameters and the control of the size of the parameters correction factor will also be investigated as means to control instability and uniqueness. Finally, the Marquardt method for unconstrained minimization is modified to include constraints and step size correction of the parameters. The resulting algorithm will be applied to solve the groundwater flow problem stated in Chapter 4.

ELEMENTS OF FUNCTIONAL MINIMIZATION

The identification of model parameters should start with the selection of an appropriate mathematical expression of the physical system's behavior in terms of the parameters. A general form of the type of constrained optimization problems in this chapter is to minimize (or maximize) some scalar function (linear or nonlinear) of a vector:

$$y = f(x) = f(x_1, x_2, \ldots, x_n) \tag{3.1}$$

subject to sets of constraints, expressed as functions of a vector:

$$\left.\begin{array}{l} g(x)\ \{=, \leq, \geq\}\ b_i\ ,\ i=1,2,\ ...,\ m \\ x \geq 0 \end{array}\right\} \qquad (3.2)$$

where:

y is a N-dimensional vector of system outputs

x is a n-dimensional vector of system inputs

g is a set of linear or nonlinear functions of x

The objective of the identification problem is to estimate b so that the deviation between the model and system responses to the input vector x is minimized according to a specified error criterion. The choice of an error criterion function, E(b), depends on factors such as type of model representing the physical system, quantity and quality of the inputs, probability distribution of the errors, sensitivity of the parameter with respect to the error criterion function, and the goal of the identification process. Classic examples of such error criterion functions are the least squares, sum of absolute errors, and the minimax error criteria.

The least squares norm is the error criteria most widely used in parameter estimation. Least squares norms are specially applicable when nothing is known about the probability distribution of the errors. In such case, the least squares estimates are the best linear unbiased asymptotic estimates. It is known that if the noise is considered random (i.e., gaussian and additive in nature), then for linear systems, the maximum likelihood a posteriori and the least squares estimates are the same [Bard, 1974].

A more general approach is to construct the objective function of residuals in a similar manner as the least squares function but with the exponent 2 replaced by p, an even integer. This is known as least p-th minimization. Large values of p emphasize the residuals that represent the greater errors. This tends to equalize the errors but only as much as the mathematical model will tolerate. Also, values of p in excess of about 20 will cause computational problems such as numerical overflow in most computers.

The sum of absolute errors norm is also a popular form of objective function which in many applications can yield more robust estimates than least squares norms. This norm is particularly suitable in optimization problems where variations in the observation data are fairly uniform.

Particularly applicable when less weighting to large errors is desirable, the minimax criterion tends to produce more conservative estimates than the least square criterion. This criterion minimizes the maximum residual in the sample space. In this method, adjustments to the variables are made only after scanning all the discrete points in the sample space to find the maximum residual. This sequence of adjustments usually results in different sample points being selected as the optimization proceeds; therefore, the objective function is not continuous. Quite often, the least squares solution is "close" to the minimax solution, and only a small additional effort is required to find it. However tempting it may be to use the absolute value of the residual, it is wise to avoid it because of its discontinuous effect on derivatives. For this reason, least squares are preferable over minimax criteria when the objective function is desired to be a smooth function. A final comment on minimax criteria is that minimax and maximum likelihood estimates are the same when the errors are uniformly distributed [Bard, 1974].

Mathematically, an error criterion function can be written as:

$$E(b) = \| \, y - \hat{y} \, \| \tag{3.3}$$

where $\| \bullet \|$ denotes a given norm and the symbol ^ a known observed value. With a given error norm, the identification problem can be expressed as:

$$\underset{b}{\text{Min}} \; E(b) \tag{3.4}$$

subject to the constraints (3.2).

In the groundwater parameter identification problem, the head distribution is represented by f(x) = h(x,y,t:T) and the constraints are boundary and initial conditions. Then, the least squares norm of the output is given by:

$$E(T) = \int_0^t \int_\Omega [\, h(x,y,t;T) - \hat{h}(x,y,t) \,]^2 \, d\Omega \, dt \tag{3.5}$$

where T are the unknown transmissivities, h(x,y,t;T) and $\hat{h}(x,y,t)$ are the calculated and observed heads respectively at various points in space and time. In general, head observations are available at t discrete values of time at n discrete observation points. Thus the discrete form of (3.5) is:

$$E(b) = \sum_{j=1}^{t} \sum_{i=1}^{n} [\, h_{ij} - \hat{h}_{ij} \,]^2 \tag{3.6}$$

where $h_{ij} = h(x_i, y_i, t_j; T)$ and $\hat{h}_{ij} = \hat{h}(x_i, y_i, t_j)$, i = 1, 2, ..., n; j = 1, 2, ..., t .

The final step for the formulation of the parameter identification problem is the selection of a computational procedure that adjusts the parameter values so that the error norm is minimized.

UNCONSTRAINED MINIMIZATION

The most commonly used algorithms for minimizing a function f(x) with respect to a vector of inputs x proceed by iterative refinements. If the function is sufficiently regular, its expansion in Taylor series can be used to produce efficient algorithms that converge to a local minimum. These methods are known as gradient methods because they require the evaluation of the derivatives of the function f with respect to x. In this classification fall all steepest descent methods, conjugate gradient methods, and all Newton-type methods.

Steepest descent methods are generally not efficient in terms of rates of convergence for many types of problems. This method starts at some initial point x_o and moves from point x_i to point x_{i+1} by minimizing along the line from x_i in the direction of the local downhill gradient $-\nabla f(x_i)$. The problem with this method is that, while moving downhill, takes alternate right angle turns, which do not, in general, lead to the minimum. An alternate way of proceeding not down the new gradient, but in a direction that is somehow constructed to be "conjugate" to the old gradient, and, insofar as possible, to all previous directions traversed. Methods which use this way of path construction are called conjugate gradient methods. Among the most important conjugate gradient methods are the Davidon [1959], Fletcher and Powell [1963], and the Polak-Ribiere [1971] methods. These methods are in general more efficient than the steepest descent methods but they still require the evaluation of derivatives which may be laborious or practically impossible for some problems. Among the methods of minimization which do not require the evaluation of the derivatives, also known as direct search methods, are the algorithms by Rosenbrock [1960]; the simplex minimization method by Nelder and Mead [1965]; conjugate directions method by Smith [1962]; and random search methods by Matyas [1965], and Shumer [1968]. In general, these methods require more computational effort than

the gradient methods and the number of function evaluations in a particular problem can make its application prohibitive. One advantage of these methods is that they are more suitable to find the global minimum in a problem with several local minima.

Particularly suitable to least squares function minimization is the Gauss-Newton method which has demonstrated to be more rapidly convergent than the steepest descent method [Traub, 1964] and the Marquardt method [Marquardt, 1963] which has found a wide range of applications in parameter estimation problems [Garay, 1976; Cooley, 1979; Sadeghipour, 1984].

The type of objective function in any minimization problem plays a very important role in determining the approach to be used to locate the optimum solution. Consider our general model described by equations 3.1 and 3.2 which for notation simplicity will be rewritten as $y = f(x)$ subject to $g(x)$ $(\leq, =, \geq)$ c. If the objective function $f(x)$ is a convex function over a constraint set of $g(x) \leq 0$, then any local minimum of $f(x)$ satisfying the constraint set will be a global minimum. However, for most practical identification problems it is very difficult to determine the global optimality conditions of the objective function. Hence, most practical minimization methods are designed to locate at least local minima. A local minimum at a point x^o must satisfy the condition $f(x^o) \leq f(x)$. In order to determine the necessary and sufficient conditions for finding a local minimum of a nonlinear function we will use a Taylor series expansion of the form:

$$f(x) = f(x^o) + [\ \nabla f(x^o)]'\Delta x + \tfrac{1}{2}(\Delta x')\ H(x^o)\Delta x + \ldots\ ] \tag{3.7}$$

where $\nabla f(x^o)$ is the gradient vector and $H(x^o)$ is the Hessian matrix of $f(x)$ defined as:

$$\nabla f(x^o) = \left(\frac{\partial f(x^o)}{\partial x_1} \quad \frac{\partial f(x^o)}{\partial x_2} \quad \ldots \frac{\partial f(x^o)}{\partial x_n} \right)^T \tag{3.8}$$

$$H(x^o) = \begin{pmatrix} \frac{\partial^2 f(x^o)}{\partial x_1^2} & \frac{\partial^2 f(x^o)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x^o)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x^o)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x^o)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x^o)}{\partial x_2 \partial x_n} \\ . & . & \cdots & . \\ . & . & \cdots & . \\ . & . & \cdots & . \\ \frac{\partial^2 f(x^o)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x^o)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x^o)}{\partial x_n^2} \end{pmatrix} \tag{3.9}$$

In order for x^o to be the location of the minimum, any point in the neighborhood of x^o must satisfy the inequality condition $f(x^o) \leq f(x)$. At a minimum, the gradient vector $\nabla f(x^o)$ must be equal to zero because each element of the Δx vector may consist of either plus or minus elements. The necessary condition for a minimum is:

$$\nabla f(x^o) = 0 \tag{3.10}$$

This means each element of the gradient vector; $\partial f(x^o)/\partial x_i$, $i = 1, \ldots, n$; must be equal to zero. If the Hessian matrix is positive definite, the sufficient condition for a minimum $f(x^o) \leq f(x)$ is satisfied. A nonlinear function that satisfies the condition of a positive definite Hessian matrix is a convex function. A drawback of using the necessary condition $\nabla f(x^o) = 0$ to determine local minima is the difficulty of solving numerically the resulting system of nonlinear equations.

In general, iterative search methods find the solution through a procedure of the form:

$$x^{(k+1)} = x^{(k)} + \alpha^{(k)} x^{(k)} \tag{3.11}$$

where $\alpha^{(k)}\, x^{(k)}$ is a correction factor applied to the current solution x at iteration k. The procedure starts at an initial guess x^o at k = 0. If a value of $x^{(k)}$ satisfies the expression $f(x^{(k)}) = 0$, a minimum has been located. Generally speaking, $x^{(k)}$ will not strictly satisfy the equality condition $f(x^{(k)}) = 0$. Instead, a condition such as $|h(x^{(k)})| < \varepsilon$ is used, where ε is a tolerance interval. This general procedure of testing and estimating is common to all iterative search methods.

The Gauss-Newton Method and Mardquardt's Modification

Methods of minimization of nonlinear functions based on the Gauss-Newton algorithm [Hartley, 1961; Bard 1974; Draper and Smith 1981; Cooley and Naff 1985] has previously been applied to the groundwater inverse problem [Yoon and Yeh, 1976; Yeh and Yoon, 1976; Gavalas et al., 1976; Cooley, 1977; Sadeghipour and Yeh, 1984].

The quasi-newton methods fall in the category of gradient methods. For gradient methods, equation (3.11) can be written as:

$$x^{(k+1)} = x^{(k)} + \delta_p^{(k)}\, R^{(k)} \tag{3.12}$$

where $R^{(k)}$ is a direction vector and $\delta_p^{(k)}$ is an appropriately selected scalar representing the step size at iteration k. Gradient methods of optimization differ basically in the form in which the vector of corrections δ_p is represented. The solution vector δ_p can be found using an equation of the form:

$$[A]\,\{\delta_p\} = \{g\} \tag{3.13}$$

where A is a nxn direction matrix and g is a vector function of x. Different gradient methods are obtained from equation 3.13 depending on the choice for the matrix A. For example, for the steepest descent method A = I, where I is the identity matrix. Similarly, if A = H where H is the Hessian matrix, we obtain the Newton method. These two methods have found only limited application on the area of parameter estimation because of severe limitations which made them computationally inefficient. Among these limitations, we can mention unreasonable convergence rates, and the required evaluation of the gradient vector and Hessian matrix at each iteration.

The Gauss-Newton method was the first to exploit the special structure of the Hessian matrix and gradient vector which occurs with least squares problems. For this case, the sum of squares nonlinear function can be represented as:

$$F(\beta) = \sum_{i=1}^{m} [\, f_i(b) \,]^2 \tag{3.14}$$

whose gradient vector $g(\beta)$ and the Hessian matrix $H(\beta)$ are:

$$g = 2\, J^T f \tag{3.15}$$

$$H = 2\, [\, J^T J + B \,] \tag{3.16}$$

where J is the mxn Jacobian matrix of f whose i-th row is given by:

$$\nabla f_i = (\partial f_i / \partial b_1 , \partial f_i / \partial b_2 , \ldots , \partial f_i / \partial b_n) \tag{3.17}$$

and the matrix B by:

$$B = \sum_{i=1}^{m} f_i H_i \tag{3.18}$$

As in Newton's method, a special form of the Hessian matrix can be obtained when minimizing a sum of squares of nonlinear functions. This expression can be written as:

$$A\ \delta_p = g \tag{3.19}$$

where:

$A = J^T J + B$

$g = - J^T f$

δ_p = vector of parameter corrections

The virtue of the Gauss-Newton method stems from the fact that this method neglects the second-derivative matrix B, thus the matrix A in equation 3.19 becomes:

$$A = J^T J \tag{3.20}$$

It is known that the Gauss-Newton method will ultimately converge at the same quadratic rate as Newton's method even though only first derivatives are required to compute H [Gill et al., 1978]. This convergence can be achieved only if J has a full column rank. Ill-conditioning of the inverse problem can cause rank deficiency in J and the method will fail to produce a stable solution.

Some of the difficulties encountered during minimization of nonlinear functions have been overcome by modifications to the Gauss-Newton Method. The Marquardt method [Marquardt, 1963] was designed to guarantee the positive definiteness of the direction matrix A. This algorithm performs an optimum interpolation between the Taylor series and gradient methods, based on the maximum neighborhood in which a truncated Taylor series gives an adequate representation of the nonlinear model. This method has been used to compensate for a high degree of collinearity among the parameters. Marquardt's method is known to produce biased estimates of the parameters. Using a mean squared error criterion which takes into account both bias and variance, the Marquardt modification is generally preferable to the unbiased estimate from the Gauss-Newton method [Marquardt, 1970]. The motivation of this method is based on the fact that ill-conditioning of the matrix A may occur by chance at any stage of the search if partial derivatives with respect to one parameter should become much smaller than those with respect to another. One mean for reducing this difficulty is by searching with a more general gradient. The Newton-Raphson vector of the form:

$$\delta_p = -A^{-1} g \tag{3.21}$$

where:

$$A = [J^T J + C]$$

$$g = J^T f$$

Here, J, C, and f are functions of β, C is a square matrix used to accelerate convergence, avoid singularities, or alleviate whatever other difficulty seems relevant.

The Marquardt method, like all gradient methods, is not scale invariant, thus by scaling the parameters β_i in units of the roots-sums-of-squares of the derivatives $\partial f_i/\partial \beta_i$ over the data set and by making $C = \mu I$, equation 3.21 can be rewritten as:

$$\delta_p = - [A + \mu I]^{-1} \; g \tag{3.22}$$

where the matrix A and the vector g have the same meaning as in (3.21), μ is a finite positive scalar, and I is the identity matrix. This scaling device places ones along the diagonal of the A matrix and standardizes the nondiagonal terms with respect to their correspondent diagonal entry, thus the computational properties of the algorithm are enhanced by reducing the scatter among the matrix entries. After scaling matrix A and the vector g, the iterative form of (3.21) at iteration k, can be written as:

$$[S^{(k)} + \mu^{(k)} I] \, \delta_p^{(k)} = g_S^{(k)} \tag{3.23}$$

where:

$$S = (s_{ij}) = \frac{a_{ij}}{\sqrt{a_{ii}}\sqrt{a_{jj}}}, \qquad g_S = (g_{Si}) = \frac{g_j}{\sqrt{a_{jj}}}$$

In equation (3.23), μ must be chosen such that the values of the objective function from successive iterations always decrease, that is $F(b)^{(k+1)} < F(b)^{(k)}$. At iteration (k+1) the updated estimates of β, b, are given by:

$$b^{(k+1)} = b^{(k)} + \delta_p^{(k)} \tag{3.24}$$

This equation is successively applied until an error criterion for convergence is satisfied. The Marquardt method is a special case of the Gauss-Newton method when

$\mu = 0$. Conversely, as $\mu \to \infty$, the orientation of δ_p approaches that of g of the steepest-descent method. Thus, Marquardt's vector combines the better features of both steepest-descent and the Gauss-Newton search through a single blend parameter μ, while ignoring the question of vector length for the steepest-descent vector. Regarding the selection of μ, Marquardt suggests to stay as close as possible to the Gauss-Newton vector by choosing small values of μ. The algorithm determines these heuristically. He gives only passing note to his ability to avoid Gauss-Newton singularities. For by making μ sufficiently large, enough weight is added to the diagonal of A to allow an inversion without numerical difficulty.

In practical applications, some of the difficulties of selecting a proper value of $\mu^{(k)}$ have been overcome by Cooley and Naff [1985] who developed a methodology to select not only the value of $\mu^{(k)}$, but also a convergence acceleration parameter $\rho^{(k)}$. This parameter is applied to the correction vector $\delta_p^{(k)}$ to avoid the problem of overshooting or undershooting. Overshooting occurs when the parameter correction vector $\delta_p^{(k)}$ has a favorable orientation but is much longer than an ideal value. The result is that the new set of parameters $b^{(k+1)}$ is almost as far (or even farther than) the old set $b^{(k)}$ from the optimum value. Overshooting is detected by large oscillations with accompanying changes in sign of components $\delta_p^{(k+1)}$ from one iteration to the next. Undershoot occurs when $\delta_p^{(k+1)}$ is too small, and it manifests itself as small steps $\delta_p^{(k+1)}$, the components of which usually do not change sign. This acceleration factor modifies equation (3.23) as follows:

$$b^{(k+1)} = b^{(k)} + \rho^{(k)} \delta_p^{(k)} \tag{3.25}$$

In (3.24) $0 \le \rho^{(k)} \le 1$ when overshoot occurs and $\rho^{(k)} > 1$ when undershoot occurs.

The theoretical basis of the modified Marquardt method of minimization of nonlinear functions is presented in detail in Appendix I.

CONSTRAINED MINIMIZATION

Instability and divergence of the solution during the application of minimization methods of the Gauss-Newton type particularly in field applications where noise in the head data and other sources propagate during the solution. One way of dealing with this problem is to incorporate into the solution prior information about the parameters. Prior information about the parameters can be in the form of exact values of certain parameters or a valid range of values defined by upper and lower bounds. In the first case when exact prior information about certain parameters is available, this information can be expressed in the form of a set of linear equalities and added to the minimization problem as equality constraints. Then if, for instance, the least squares criteria is used, Lagrangian techniques can then be used to solve the minimization problem.

However, exact information about parameters is almost never found for field problems making necessary the employment of alternative methods to incorporate field prior information into the solution. In practice, this has been accomplished by a range of parameter values that lie between some upper and lower bounds. This information can be translated into inequality constraints and incorporated into the unconstrained problem. Introducing prior information in the form of inequality constraints biases the estimates, favoring parameters with narrower feasibility region.

Inequality Constraints

During the application of optimization methods, it is often desirable for the parameters to have an admissible range of values. Prior information about the

parameters obtained from geologic information or field measurements can be incorporated into the solution process by means of inequality constraints. These constraints define the feasible region for each parameter by means of an upper and lower bound. Mathematically, parameter constraints can be represented by:

$$bmin_j \leq b_j \leq bmax_j \tag{3.26}$$

where $bmax_j$ and $bmin_j$ represent the maximum and the minimum admissible values for the parameter b_j. It is known that the estimates from constrained minimization are unbiased estimates and more accurate than the parameters from unconstrained minimization, depending on the amount and accuracy of the prior information.

The range of permissible values in inequality constraints should be established from field data such as field measured transmissivities from pump tests and core analyses. The range of the values on each estimate should be a function of the reliability of the field measurements, even for applications where only low reliability estimates are available. For instance, the application of a lower bound on the parameters, can prevent the estimates from becoming negative.

Lagrange Multipliers

The general form of the constrained optimization problem involves constraints on the objective function, that is, the minimization of f(x) subject to h(x) = 0 and c(x) $\geq$ 0. If some of the inequality constraints are not "binding," or inactive, they can be ignored, since they are satisfied. The essential part of the constrained problem is to deal with the equality or active constraints. One of the requirements for ensuring that that a critical point is a global optimum is that the constraints be a convex set. A

constraint set is defined to be convex if any two point in the set falls within the boundary of the set.

A convenient method to handle active constraints is the method of Lagrange multipliers. This method avoids the transformation and direct substitution into the objective function. By introducing a new variable, the Lagrange multiplier λ, the constrained optimization model can be rewritten as an unconstrained problem. This new model is called a Lagrange function which for a model of m active constraints can be defined as:

$$L(x,\lambda) = f(x) + \sum_i \lambda_i (b_i - g_i(x)) \tag{3.27}$$

The necessary condition for a local minimum is:

$$\left.\begin{aligned} \nabla L_x &= \frac{\partial L}{\partial x} = 0 \\ \nabla L_\lambda &= \frac{\partial L}{\partial \lambda} = 0 \end{aligned}\right\} \tag{3.28}$$

Since there are n control variables x, and m constraint equations, there are n + m equations in the solution set.

$$\left.\begin{aligned} \frac{\partial L}{\partial x_j} &= \frac{\partial f(x)}{\partial x_j} - \sum_{i=1}^{n} \lambda_i \frac{\partial g_i(x)}{\partial x_j} = 0, \quad j = 1, 2, \ldots, n \\ \frac{\partial L}{\partial \lambda_i} &= b_i - g_i(x) = 0, \qquad\qquad i = 1, 2, \ldots, m \end{aligned}\right\} \tag{3.29}$$

The condition that $\partial L/\partial \lambda = 0$ ensures that the sets of all active constraint equations are satisfied.

Kuhn and Tucker extended the concepts of Lagrange multipliers for models that include active and inactive constraints. Their general model has the form:

$$\left.\begin{array}{l} y = f(x) \\ g_i(x) \le b_i\,; \;\; i=1,2,... \\ g_k(x) \ge b_k\,; \;\; k=1,2,... \\ g_m(x) \ge b_m\,; \;\; m=1,2,... \\ x \ge 0 \end{array}\right\} \qquad (3.30)$$

For this model the Lagrange multiplier equation is:

$$L(x,\lambda,\mu,\upsilon) = f(x) + \sum_i \lambda_i(b_i - g_i(x)) + \sum_k \mu_k(b_k - g_k(x)) + \sum_m \upsilon_m(b_m - g_m(x)) \qquad (3.31)$$

where λ, μ, and υ are the control variables associated with the three types of constraints: less-than-or-equal-to, greater-than-or-equal-to, and equality constraints, respectively. The necessary condition for a critical point is:

$$\nabla_x L = 0, \qquad \nabla_\lambda L = 0, \qquad \nabla_\mu L = 0, \qquad \nabla_\upsilon L = 0 \qquad (3.32)$$

The approach for establishing critical points is the same one utilized for the case of active constraints only. However there are additional factors that must be considered.

These additional conditions are known as Kuhn-Tucker necessary and sufficient conditions for a global minimum of the general problem (3.30) with Lagrange multiplier (3.31). These conditions are summarized as follows.

$$
\left.
\begin{array}{l}
1.\quad x_j \geq 0 \quad \text{and} \quad \dfrac{\partial L}{\partial x_j} \geq 0 \\[2ex]
2.\quad (a)\quad \text{if } \lambda_i = 0, \text{ then } b_i - g_i(x) \geq 0 \quad \text{(inactive constraint)} \\
\qquad (b)\quad \text{if } b_i - g_i(x) = 0, \text{ then } \lambda_i \leq 0 \quad \text{(active constraint)} \\[2ex]
3.\quad (a)\quad \text{if } \mu_k = 0, \text{ then } b_k - g_k(x) \leq 0 \quad \text{(inactive constraint)} \\
\qquad (b)\quad \text{if } b_k - g_k(x) = 0, \text{ then } \mu_k \geq 0 \quad \text{(active constraint)} \\[2ex]
4.\quad \nu_m \text{ is unrestricted in sign, } -\infty \leq \nu_m \leq \infty \text{ and } b_m - g_m(x) = 0 \\[2ex]
5.\quad f(x) \text{ is a convex function} \\[2ex]
6.\quad (a)\quad g_i(x) \text{ is a convex function} \\
\qquad (b)\quad g_k(x) \text{ is a concave function} \\
\qquad (c)\quad g_m(x) \text{ is a linear function}
\end{array}
\right\} \quad (3.33)
$$

Any critical point found can be tested to determine if it is a global optimum. Conditions 1 to 4 are the necessary conditions for a global optimum; thus one may use them to establish critical points. If conditions 5 and 6 are satisfied, the critical point is a global optimum.

The lack of accurate field data in most practical problems, limit the nature of the type of constraints to inequality constraints. This means that only a range of values can be assigned to the parameters. Because of the inequality nature of these constraints, the Lagrangian approach is not longer applicable. For problems with

inequality constraints of the kind defined by (3.26) algorithms such as the penalty method for linear and nonlinear constraints [Carroll, 1961] and gradient projection methods [Rosen, 1960] can be applied to include upper and lower bounds on the parameters. These methods can only guarantee a feasible minimum.

Penalty Function Method

In the penalty function method the objective function is modified by p terms, one for each parameter. The i-th penalty term is selected such a way that it has a negligible value in the interior of the feasible region but increases drastically when it approaches the i upper or lower bound. This method will not be adequate when the minimum is located on one of the bounds or when heavily weighted penalty terms prevent convergence. The Rosen method does not modify the objective function, instead this method modifies the optimization algorithm and carries out the solution as an unconstrained problem until a bound is found in the search direction. Then the negative gradient direction is projected back onto the intersection of the active constraints and the search continues on this projected direction. The conditional convergence is achieved when the projected vector becomes zero.

The method of penalty function can be easily incorporated into Marquardt's algorithm. To accomplish this, the least squares objective function (3.6) is modified in such a way that it remains almost unchanged in the interior of the feasible region bounded by the upper and lower values of each parameter. As the solution approaches the constraints, the penalty function term applies a large value to the modified objective function increasing drastically its value. This is done by applying a penalty function to each inequality constraint. This function is nearly zero when the constraint is strongly positive, but increases sharply as the constraint function

approaches zero from above. This method of imposing linear constraints assigns a penalty function to the constraint $c_j(b) \geq 0$ of the form:

$$\zeta(b) = \frac{\gamma_j}{\Psi_j(b)} \tag{3.34}$$

where γ_j is a small positive constant. Including these new terms into an objective function $\Phi(b)$ would yield a new objective function of the form:

$$\Phi(b)' = \Phi(b) + \zeta(b) = \Phi(b) + \sum_{j=1}^{2p}\left(\frac{\gamma_j}{\Psi_j(b)}\right) \tag{3.35}$$

where p is the number of parameters. There are two terms $(\gamma_j)/\Psi(b)$ for each parameter because for each constraint reflecting the bounds $bmin_j \leq b_j \leq bmax_j$, an equivalent form can be expressed by two equality constraints of the form:

$$\left.\begin{aligned} \Psi_j(b) &= bmax_j - b_j > 0 \\ \Psi_{j+1}(b) &= b_j - bmin_j > 0 \end{aligned}\right\} \tag{3.36}$$

Bard [1974] suggests setting the values of γ_i and γ_{i+1} as follows:

$$\gamma_j = \gamma_{j+1} = .001(\, bmax_j - bmin_j\,)\, \Phi(b) \tag{3.37}$$

If the current parameters at iteration k, $b^{(k)}$, are well in the interior of the feasible region, a good choice of γ_j , according to Bard [1974], would be:

$$\gamma_j = .001\ \Psi_j(b^{(k)})\ \Phi(b^{(k)}) \tag{3.38}$$

Selected Algorithm for Functional Minimization

After reviewing the most common difficulties encountered in the groundwater parameter identification problem and the different methods used in the literature for optimization problems, it is appropriate, at this point, to select the most adequate techniques for the solution of our problem. It was concluded in Chapter 2 that the optimization approach was a better approach given the limitations in data quality and quantity for most practical problems. Optimization algorithms often fail in practical groundwater parameter identification, mainly because of overparameterization or ill-conditioning of the matrices involved in the solution. In this section we will propose an optimization algorithm which includes devices specifically designed to overcome some of the most serious problems related to ill-conditioning during the optimization process.

The optimization algorithm will be based on the minimization of the least squares error norm (3.6) and the minimization of this function will be carried out by using a modified version of Marquardt's algorithm to avoid singularities in the direction matrix A. The problem of overshooting or undershooting of the solution will be controlled by a step correction factor, ρ. Prior information on the parameter will be included in the solution as inequality constraints. These inequality constraints will be easily incorporated into the objective function by the penalty method [Carroll, 1961]. In the next chapter we will discuss the ill-effects of overparameterization and how this problem will be handled by reducing, during the minimization process, the dimension of the parameter space to a level compatible with the quantity and quality of the available data. This process of parameterization of the zonal transmissivities is based on the selection of the model with the greatest sensitivity among all possible models resulting from the combination of ill-defined parameter zones with their neighboring zones.

CHAPTER 4

INVERSE SOLUTION FOR STEADY STATE CONDITIONS

This chapter is about the formulation of the mathematical model and presentation of the techniques used in the solution of the groundwater parameter identification problem. The aquifer under consideration is inhomogeneous under confined steady state conditions. The aquifer parameters subject to identification are the transmissivities, since for steady state problems the aquifer storativity drops out of the governing flow equation. The identification problem is formulated based on the least squares optimization method presented in Chapter 3. The functional representation of the head distribution will be obtained using the finite element method. The sensitivity coefficients required to evaluate the Jacobian matrix will be obtained by the sensitivity equation method. The problem of overparameterization, is solved with the parameter zonation approach. For this purpose, a zonation algorithm is presented as an integral part of the optimization procedure and is aimed to reduce the number of ill-defined parameters which can lead to ill-conditioning of the sensitivity matrix. When ill-defined parameters are eliminated from the solution, it is expected that this reduced set of parameters leads to a more stable solution.

GROUNDWATER INVERSE PROBLEM DEFINITION

The aquifer of interest in this study is assumed to be inhomogeneous and isotropic. The fluid, which is assumed to be of single phase and incompressible, flows between two impermeable strata under confined conditions, and there are no spatial variations of the head distribution in time (i.e., steady state). The vertical component of the flow is assumed negligible, also, for the steady state case, the

observation data at a particular location is an average value over a long period of time.

The application of a mathematical model to practical problems will inevitable lead to errors. These errors are due to the inability of the model to accurately represent the actual field conditions and numerical approximations involved in the solution. As previously discussed, these errors contribute to the ill-posedness of the inverse problem in an unpredictable way mainly because of the inability of the optimization methods to properly weight the source of error. To this date, numerical approximations are the only form of solution of the groundwater flow equation for most practical problems and, for the inverse problem, modeling errors will always be a part of the problem. Therefore, it is common practice to assume that the only modeling errors are due to roundoff and domain discretization.

For parameter identification purposes, only the transmissivity will be considered in this study, although other parameters such as boundary conditions, net recharge or discharge, and for transient problems, the storage coefficient or initial conditions can also be identified with the proposed methodology.

The aquifer transmissivity, defined as the rate at which the fluid is transmitted through the aquifer per unit width under a unit hydraulic gradient, is assumed to vary spatially over the entire domain but independently of the direction of measurement. However, for parameter zonation purposes, the transmissivity will be assumed to be constant over a particular zone but may vary from zone to zone.

The partial differential equation which describes the two-dimensional movement of water through a confined aquifer under steady state conditions is given by the following equation [Jacob, 1950; Bear, 1979]:

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right)=Q \tag{4.1}$$

such that

$$h(x,y) = f_1(x,y) \qquad x,y \in \partial\Omega_1 = \Gamma_1$$

$$\frac{\partial h}{\partial n} = f_2(x,y) \qquad x,y \in \partial\Omega_2 = \Gamma_2 \tag{4.2}$$

where:

h	= h(x,y)	=	head potential
T	= T(x,y)	=	aquifer transmissivity
Q	= Q(x,y)	=	external stress (source or sink)
x,y	=		spatial coordinates
Ω	=		aquifer domain
n	=		normal direction to the boundary
Γ	= $\partial\Omega$	=	domain boundary
f	= f(x,y)	=	known boundary function

Traditionally, the forward solution of equation 4.1 for the head distribution h(x,y) subject to the boundary conditions (4.2) is accomplished by the finite difference, finite element, or the boundary integral method. In either case, the solution of (4.1) requires the exact distribution of T and Q. For most practical problems, the flow term Q is assumed known, including areal recharge, and point or sink discharges as well as the boundary conditions on the portions of the aquifer Γ_1 and Γ_2. On the other hand, the groundwater parameter identification problem involves determining the distributed parameters, T, which characterize the aquifer, based on observations of pumping and recharge wells (Q), boundary flows, and water levels at observation wells.

It is obvious that the inverse problem should be solved before a model can be successfully utilized for its legitimate purpose. One way is to use modeling experience, objectivity, and prior geological information. A more formal

development has been hampered because of the ill-posedness characteristics of the inverse problem. Although it is apparent that in any practical application, the problem should always be properly posed in the physical sense, unfortunately, in the usual mathematical formulations, the inverse problem is inherently ill-posed mainly because of insufficient or inaccurate field data, and because of different combinations of parameters, boundary conditions, or discharge/recharge values which may produce the same head distribution thus giving raise to nonuniqueness. Insufficient informative data relative to the number of parameters will inevitably lead to a physically underdetermined system.

The inclusion of informative and accurate prior information on the parameters, boundary conditions, or discharges can be effectively used to alleviate some of the problems related to nonuniqueness, but in most practical field problems, the gathering of this kind of prior information may become difficult and economically unfeasible. Ideally, a sampling program to collect field information on the heads, parameters and boundary conditions should take place to provide sufficient data for a well-posed inverse problem. However, the problem of locating the observation wells arises when trying to collect head data which is sensitive to all the parameters. The optimum determination of the location and amount of field data for inverse problems is a difficult problem and has evolved into a whole class of problems called field or sampling design [St. John and Draper, 1975; Knopman and Voss, 1987; Casman, Naiman, and Chamberlain, 1988; Nishikawa and Yeh, 1989; Knopman and Voss, 1989; Yeh and Sun, 1990].

FORMULATION OF THE IDENTIFICATION PROBLEM

The head potential over a two-dimensional inhomogeneous aquifer under confined and steady state conditions is given by equation (4.1). The main objective of

the parameter identification is to determine the transmissivity function T using available head potential information at scattered points within the aquifer domain in addition to boundary flow, areal recharge, and point source/sink information.

An optimization approach is used to find a feasible solution by minimizing an error criterion defined as the sum of square errors between the observed heads, $\hat{h}$, and the computed head values, h, as follows:

$$\min \Phi(x,y;T) = \sum_{i=1}^{n} [\, h(x_i,y_i;T) - \hat{h}(x_i,y_i) \,]^2 \tag{4.3}$$

Prior information on the parameters from geologic data, pumping tests, or core analyses may be incorporated into the solution to keep the parameters within a range of feasible values. Upper and lower bounds in the parameters are imposed during the minimization as inequality constraints of the form:

$$Tmin_j < T_j < Tmax_j \tag{4.4}$$

To control overparameterization during the identification of the transmissivities, the dimension of the parameter space must be adjusted with respect to the amount of informative data provided by the observed heads. For this purpose, parameterization of the parameter space during optimization is applied to reduce the number of unknown parameters during the solution of a parameter identification problem. Generally speaking, parameterization can be performed on a vector of parameters T_p of p parameters to produce a vector T_m of m parameters, where $m < p$, by means of a matrix

$$G = (\vec{g}_1, \vec{g}_2, \ldots, \vec{g}_m) \tag{4.5}$$

where the vectors $\vec{g}_i$ are a set of suitable orthonormal vectors [Gavalas et al., 1976]. Using the matrix G of order pxm the parameterization of the vector T_p is then given by:

$$T_m = G\, T_p \tag{4.6}$$

There are two basic parameterization approaches found in the literature: the zonation and the interpolation approaches. The zonation approach reduces the number of parameters by forming subregions on which the parameter in question holds a constant value. This approach is the simplest and easiest to apply and is particular applicable when prior information on the zonal distribution of the parameters is available from geological information [Yeh and Yoon, 1976; Cooley, 1977; Neuman and Yakowitz, 1979]. The popularity of this method is due mainly to the widespread use of finite difference and finite element models used to obtain forward solutions for the heads in which the parameters are provided by gridded zones or groups of finite elements. Among these models are the U.S.G.S. 2-D and 3-D models [McDonald, Harbaugh, 1984; Trescott, Pinder and Larson, 1976].

In the interpolation approach of parameterization, the transmissivity function is assumed to be a continuous function of the spatial coordinates x and y and is usually represented by piecewise polynomials [Distefano and Rath, 1975; Garay et al., 1976; Yeh and Yoon, 1981]. This method has the advantage over the zonation approach of representing the transmissivity field as a smooth function and not as a step function with sharp variations on the zone boundaries. However, because of the smoothing effect of the interpolation functions, the interpolation approach may have

difficulties when applied to aquifers with large transmissivity variations over short distances or a sudden change in transmissivity due to a geologic feature.

When parameterization by zonation is chosen to reduce the number of parameters, the matrix G of order pxm, also known as the amalgamation matrix [Aitchison, 1986], has m elements equal to 1, one on each row and at most one in each column, and the remaining m(p-1) elements equal to zero. The parameterization of the transmissivity vector T_p applied during the minimization of the objective function (4.3) can be rewritten as:

$$\Phi = \sum_{i=1}^{n} [\, h(x_i,y_i;GT_p) - \hat{h}(x_i,y_i) \,]^2 \qquad (4.7)$$

For minimization with Marquardt's algorithm, equation (3.19) can now be written as:

$$[\, G^T A G \,] \, \delta_{p-1} = G^T g \qquad (4.8)$$

Equation (4.8) is now solved for the reduced set of corrections δ_{p-1} and a new set of parameters T is obtained at each iteration until convergence to a local minimum is achieved.

Because ill-conditioning may appear at any stage of the minimization, parameterization should be applied only when needed, from the point of view of controlling stability and eliminating nonuniqueness. If the solution process converges to a solution without noticeable instability, then the zonation could never be applied. However, parameter reduction of a converged parameter set should be investigated if it further reduces the error produced by statistical uncertainty of the parameters. This error component added to the error produced by the parameterization (which will

increase as the number of zones decreases) attains a minimum at an intermediate number of zones [Gavalas, 1976].

The problem of determining how many and which ill-defined parameters should be removed from the solution is equivalent to determining the structure of the parameterization matrix G. This problem will be solved in the next section where the structure of the covariance is studied and the singular value decomposition of the A matrix is used as a method to reduce the dimensionality of the parameter space.

STATISTICAL MEASURES OF PARAMETER RELIABILITY

In most practical groundwater modeling applications, the ill-posedness characteristics of the inverse problem may lead to large uncertainties in the identified parameters. This adverse effect makes it necessary to evaluate the reliability of the estimates so that the relative worth of the parameter set can be evaluated. The complications raised by nonlinearities in the problem, have impeded the development of practical statistical indicators applicable to nonlinear identification problems. Until now, most practical measures of parameter reliability have been implemented into non-linear least squares theory by assuming linearity of the model. When the model is highly nonlinear, these approximations may not be applicable. The degree of nonlinearity for a particular problem can be evaluated with Beale's measure of nonlinearity [Beale, 1960]. Some of the most widely used statistical measures of parameter reliability based on linear least squares theory are described in this section.

For a linear model the error variance, s^2, is an unbiased estimate of σ^2 whereas for a nonlinear model there exists bias as a result of the assumption of a linear model. However, for nonlinear cases where the degree of nonlinearity is not severe, σ^2 gives a useful measure of overall goodness of fit of the model. For σ^2 constant and

unknown, the following approximation can be used to estimate the error variance [Beck and Arnold, 1977]:

$$s^2 \approx \frac{\Phi(b)}{n - p} = \frac{\varepsilon^T \varepsilon}{n - p} \tag{4.9}$$

where n is the number of observations and p the number of parameters. The standard error of the fit is given by s. In general, $s/\Delta y$, where Δy is the difference between the maximum and minimum values of the dependent variable y, should be small.

Other important statistical measures of goodness of fit can be obtained with the aid of the covariance matrix of the parameters [Beck and Arnold, 1977]:

$$\text{Cov}(b) = P = \sigma^2 A^{-1} \approx s^2 A^{-1} \tag{4.10}$$

where P is the covariance matrix, A is the sensitivity matrix previously defined in Chapter 3 (Eq. 3.19) and s^2 is the estimated error variance.

The standard error of the estimates is a measure of the range over which the respective parameter may be varied and produce a similar solution for the dependent variable as that obtained with b. It can be computed by:

$$\text{s.e.}(b_i) = \sqrt{\text{cov}\,(b_i\,,\, b_i)} = \sqrt{p_{ii}} \tag{4.11}$$

The trace of the covariance matrix, tr[P], may also be used as a measure of overall accuracy and reliability of the estimated parameters [Sadeghipour, 1984].

A useful statistical measure that has direct application on parameter reliability, is the correlation coefficient, r_{ij} , between any two parameters b_i and b_j. This coefficient is a function of the covariance p_{ij}, and is defined as:

$$r_{ij} = \frac{Cov(b_i,b_j)}{\sqrt{Var(b_i)}\sqrt{Var(b_j)}} = \frac{p_{ij}}{\sqrt{p_{ii}}\sqrt{p_{jj}}} \tag{4.12}$$

The element r_{ij} of the correlation matrix is an indicator of the degree of linear dependence between the parameters b_i and b_j. Linearly dependent parameters cannot be simultaneously determined without leading to nonuniqueness. In practical situations, a high degree of correlation between parameters, indicated by off-diagonal values of R greater than 0.9, may give an indication of unreliable estimates.

Confidence intervals and regions can also be established on the parameters with the aid of the covariance matrix. The approximate $100(1-\alpha)\%$ confidence interval on the parameter estimate b_i is:

$$b_i \pm s.e.(b_i)\, t_{1-\alpha/2}(\nu) \tag{4.13}$$

where $t_{1-\alpha/2}(\nu)$ is the t statistic associated with $(1-\nu)100\%$ confidence region and ν degrees of freedom, usually (n-p). The confidence region for parameter b , using the F statistic, is given by:

$$(b - \beta)\, P^{-1} (b-\beta) = p\, s^2\, F_{1-\alpha}(p, n-p) \tag{4.14}$$

When applicable, these measures of parameter reliability and goodness of fit should be computed to estimate the relative worth of the estimated parameters and the validity of the regression model. Of particular usefulness in this study is the trace of the covariance matrix, tr[P], which will be used as a measure of reliability between sets of parameters of different dimensions. This comparison between different

parameter sets is a key step in the parameterization of the transmissivity space proposed in this study.

PARAMETER ZONATION USING THE COVARIANCE MATRIX

The determination of the best system structure is proposed based on the covariance matrix of the estimates. This matrix provides us with information about the parameters which are more likely to be unreliable during the identification process. With this information, one can decide which parameters to eliminate as well as the structure of the reduced set of estimates. For parameterization purposes, we will assume that the theoretical expression for the covariance matrix (4.10) is a valid approximation in the neighborhood of b, then rewriting the inverse of A as:

$$A^{-1} = \frac{\text{adj}\,(A)}{|A|} \tag{4.15}$$

where adj (•) denotes the adjoint matrix and |•| the determinant. Furthermore, the determinant can be expressed in terms of its eigenvalues as:

$$|A| = \prod_{i=1}^{p} \lambda_i = \lambda_1 \lambda_2 \ldots \lambda_p \tag{4.16}$$

In the parameter space the determinant of the covariance matrix is proportional to the volume of the confidence ellipsoid surrounding the parameter estimates [Fedorov and Pazman, 1968]. For $|A|=0$, there exists linear dependence among some of the parameters. If $|A|=0$, but not exactly zero, near linear dependence is found among some of the columns of the matrix. In this case, the spread between the eigenvalues can be very large and will increase as the smallest eigenvalue λ_1 approaches zero.

Therefore, the determinant and the inverse of the condition number of the matrix, given by λ_p/λ_1, will approach zero.

All the above statements apply to the A matrix, however, similar conclusions can be obtained for the covariance matrix. For the A^{-1} matrix, the eigenvalues are given by the inverse of the eigenvalues of the A matrix , that is $1/\lambda_1$, $1/\lambda_2$, ..., $1/\lambda_p$, and the condition number is given by λ_1/λ_p. The scaling of the computed variance s^2 will have no effect on the spread of the eigenvalues. Also, it is important to mention that the eigenvectors of the matrix $A = (\vec{e_1} , \vec{e_2} , \dots , \vec{e_m})$ are equal to the eigenvectors of the matrix A^{-1}.

In most cases of practical interest, the characteristic values, λ_i, of the matrix A decline very rapidly with increasing i as a result of spatial correlation of the aquifer properties. Therefore, parameterization can effectively be applied to the aquifer properties to reduce the statistical uncertainty on a reduced set of predicted values. If parameterization by zonation of the form given by Eq. 4.5, the matrix G can be easily defined in terms of a suitable set of orthonormal vectors such as the eigenvectors of the A matrix,

$$G = (\vec{e_1} , \vec{e_2} , \dots , \vec{e_m}) \tag{4.17}$$

where m is the number of significant eigenvalues and n-m is the number of "near-zero" eigenvalues. For this type of parameterization, Shah et al. [1978] showed that the effect of parameterization in reducing the error arising from (M - r) small eigenvalues is negligible when the rank of the sensitivity matrix A = $r < M$, where M equals the order of A. This error analysis was based on the trace of the covariance matrix of the estimates P given by:

$$\text{tr}[P] = \text{tr}[I - GG^T]\, P^* \,[I - GG^T] + \sigma^2 \sum_{i=1}^{m} \frac{1}{\lambda_i} \qquad (4.18)$$

where G is the parameterization matrix, P^* is the covariance matrix of the true parameters (assumed known), I is the identity matrix, and λ_i, i = 1,..., m are the eigenvalues of the matrix A. In equation 4.18, the first term represents the error resulting from the vector of aquifer parameters T_m having p components restricted by equation (4.5) to depend only on m parameters with $m \leq p$. This error decreases gradually as m increases and is actually zero when m = p. The second term given by the eigenvalues of the covariance matrix, depends on the sensitivity of the measurements to the transmissivities and for a given set of measurements increases rapidly with increasing m. The rate of increase of this term depends upon the spread of the eigenvalues of the covariance matrix.

By definition, the diagonal elements of the covariance matrix are variances of the estimated parameters. A large value of a variance indicates that the corresponding parameter is ill-determined. On the other hand, parameters associated with small variances are less likely to be in error. In order to remove the ill-determined parameters from the identification, it is necessary to have a measure of parameter reliability to compare alternative parameter sets of different dimensions. Among such measures, the trace of the covariance matrix or its determinant can be used to assess model reliability.

A direct comparison of the elements of the covariance matrix for sets of parameters with different dimensions is not meaningful, therefore, the following form of the covariance matrix [Yeh and Yoon, 1981] can be used to compare traces of covariance matrices of different dimensions:

$$\text{trace}\,[P_g] = \text{trace}\,[G\, A^{-1}\, G^T]\, s^2 \qquad (4.19)$$

Parameterization by zonation increases the sensitivity of certain zones by the annexation of a neighboring zone. If the zone corresponds to an ill-determined parameter, the new zonation pattern will likely produce parameters with less uncertainty at the expense of amplification of the errors during the solution. However, the new zonation pattern is chosen such that the overall sensitivity of the new model is increased and the sum of squared errors corresponding to the new zonation pattern, Φ', is less or equal to an error tolerance factor, ε'. One way to accomplish this is to compute the determinant of the sensitivity matrix and the value of the objective function, Φ, for each model obtained from the combination of the zone to be deleted with its neighboring zones. If there is a combination which leads to a model of greater sensitivity (larger determinant of the sensitivity matrix) and which also decreases Φ, then the combination is accepted, otherwise no parameterization is applied at this particular level of the optimization and the problem should be restarted at the current point in the p-parameter space.

The detection of linear dependencies among the parameters can be easily accomplished by applying singular value decomposition (SVD) to the matrix A. This technique is useful when dealing with matrices that are either singular or very close to singular [Strang, 1980]. The singular value factorization of the matrix A is:

$$A = J^T J = U W V^T \tag{4.20}$$

where U is a pxp orthogonal matrix, W is a pxp square diagonal matrix with positive or zero elements, and V^T is the transpose of a pxp orthogonal matrix. Since U and $V^T$are orthogonal, therefore $U^T U = V^T V = 1$. Furthermore, the inverse of U and V equal their transpose matrices and the inverse of W is given by the diagonal matrix

whose elements are the reciprocals of the elements w_i. Thus Eq.(4.20) for the inverse of the sensitivity matrix can be rewritten as follows:

$$A^{-1} = V\left(\text{diag}\frac{1}{w_i}\right)U^T \tag{4.21}$$

If during the minimization, a value of an eigenvalue of A, w_i, becomes zero, then there is no unique solution to the system of equations $A\,\delta_p = g$ because any vector in the null space (any column of V with a corresponding zero w_i) can be added to δ_b in any linear combination. SVD finds the solution of smallest length, $|\,\delta_p\,|^2$, among the set of solutions formed by the vectors in the nullspace by simply substituting $1/w_i$ by zero if $w_i = 0$. Then the solution vector can be computed as:

$$\delta_b = V\left(\text{diag}\frac{1}{w_i}\right)[\,U^T g\,] \tag{4.22}$$

When the matrix A is ill-conditioned, direct solution methods such as Gaussian elimination may give a solution to the system of equations. However, the solution vector may have wildly large components whose algebraic cancellation, when multiplying for the matrix A, may give a very poor approximation to the vector g. In these situations, SVD zeroes the small w's in W to eliminate a corrupted combination of equations which may pull the solution vector off towards infinity along some direction that is almost a nullspace vector.

The mxp matrix G can be easily formed by deleting from the identity matrix, I, the (p - m) columns of corresponding zero values of $1/w_i$ in W. From (4.16) and (4.21) the correction vector to the subset of parameters can be defined as:

$$\delta_p = \left(G^T V \left(\text{diag} \frac{1}{w_i} \right) G \right) [G^T U^T g] \tag{4.23}$$

The purpose of G and G^T in (4.23) is to delete the rows and columns corresponding to the zero values of $1/w_i$. These new corrections are then applied to the p-vector of parameters at iteration (k) as follows:

$$T^{(k+1)} = G\, T^{(k)} + \rho^{(k)}\, \delta_p \tag{4.24}$$

All the proposed methodologies for deleting an ill-defined parameter should only be applied during the minimization of Φ if: (1) after the step scaling factor, ρ, has failed to control overshooting or undershooting of the solution, instability persists as large oscillations with accompanying changes in the sign of components of the correction vector δ_p, (2) divergence of the solution is detected when the value of a parameter constraint is violated, or if (3) a converged set of parameters contains some parameters with large standard errors or high correlation coefficients (> 0.9).

NUMERICAL SOLUTION OF THE FORWARD PROBLEM

Several methods have been applied in the literature for the forward solution for the heads. The most popular methods are the finite difference, the finite element, and the boundary integral equation method. Finite difference and finite element methods, also known as domain methods, discretize the domain of the problem into a number of elements. The governing equations of the problem are then approximated over the region by functions which fully or partially satisfy the boundary conditions. On the other hand, boundary methods use approximation functions that satisfy the governing equations in the domain but not the boundary conditions. Finite differences have been widely used as a method of solution in groundwater hydrology

because its relative simplicity of implementation for numerical solution. This method usually approximates the solution between nodes in the space and time domains by a Taylor series expansion. A severe limitation of this method is the simplicity of the meshes used to discretize the domain. Heterogeneities of the properties can be handled provided that the shape of these heterogeneities can be adequately represented by the shape of the meshes; and anisotropy must be restricted to directions parallel to the sides of the meshes.

The finite element method is a variation of the Raleigh-Ritz method used to minimize a functional representation of a physical quantity in a problem. The finite element method provides an approximate minimization of a functional (such as the potential energy of the system). Any mathematical problem in which a stationary value of a definable functional provides the solution can be approximated by the finite element method. Techniques of minimization of weighted residuals include the Galerkin, collocation, and least squares methods. With the finite element method, the shapes of the meshes are less restricted than for a finite difference mesh. In practice, triangles and quadrilaterals of straight or curvilinear sides are used to discretize the domain while allowing one to represent more accurately the shape of the boundaries of the medium. Finite elements can also handle any directions of anisotropy in space and time.

The boundary integral equation method (BIEM) is a relatively new method of solution for groundwater problems. This method is more efficient than domain methods in the sense that the precision of the computations is not a function of the size of the elements used. However, this method requires that the properties of the medium in a given element be constant. The BIEM is therefore less flexible and general than the domain methods for highly inhomogeneous media. Brebbia presents an introduction to this method [Brebbia, 1978] and its applicability to problems in

porous media has been published by several authors [Liu and Liggett, 1979; Ligget and Liu, 1979].

Finite Element Solution Method

The finite element method has been chosen for this study not only for its advantages over the finite difference method to represent the domain's boundaries and over the BIEM for its superiority to represent inhomogeneities in the medium, but also because it is a well established, widely used technique in the area of groundwater modeling.

The minimization of an objective function by iterative methods, requires the computation of the head distribution given the transmissivities, areal recharge, nodal discharges, and boundary flows and is known as the forward problem. The solution of the forward problem consists in solving (4.1) subject to (4.2) for h = h(x,y;T). Assuming that the problem is properly posed in the mathematical sense, such a solution will always exist. This means that the spatial distribution of the aquifer parameters (transmissivities); internal and boundary flows; specified flow and constant head boundaries are known exactly.

It is obvious that most groundwater practical problems do not meet any of these conditions and estimates usually must suffice. However, it is known that reasonable estimates of the aquifer parameters and boundary conditions will yield errors in the predicted head distribution which are also reasonable and do not magnify. Furthermore, as the errors in the parameters tend to zero, so do the errors in the estimated heads.

For the forward solution to obtain the hydraulic head distribution, the following assumptions will apply: (1) the two-dimensional steady state groundwater head potential in an isotropic, inhomogeneous confined aquifer is described by Eqs.

4.1 and 4.2, (2) the transmissivity distribution is known over the entire aquifer, (3) the aquifer parameters T hold a constant value over finite areas called elements, and (4) all the internal fluxes and boundary conditions are known exactly. Under these assumptions, for a finite element e, equation 4.1 becomes:

$$\frac{\partial}{\partial x}\left(T^e \frac{\partial h}{\partial x}\right) + \frac{\partial h}{\partial y}\left(T^e \frac{\partial h}{\partial y}\right) = f \tag{4.25}$$

such that

$$\begin{aligned} h(x,y) &= h_1(x,y) \qquad x,y \in \partial\Omega_1^e = \Gamma_1^e \\ T^e \frac{\partial h}{\partial n} &= h_2(x,y) \qquad x,y \in \partial\Omega_2^e = \Gamma_2^e \end{aligned} \tag{4.26}$$

Here, T^e denotes a constant value of transmissivity in the element e. The finite element method assumes that the dependent variable in the governing equation, h, can be approximated by an expression of the form:

$$\tilde{h} = \sum_{j=1}^{n} h_j \psi_j \tag{4.27}$$

where h_j is the value of the head potential at a point (x_j,y_j) and ψ_j are linear interpolation functions with the property:

$$\psi_i(x_j,y_j) = \delta_{ij} \tag{4.28}$$

where δ_{ij} is the Dirac delta function. In the finite element method the basis functions, ψ_i, are chosen to be polynomials with a value of unity at a given node i and zero at all other nodes. These polynomial functions must also satisfy some of the boundary conditions. The accuracy of the finite element method is highly dependent on the choice of these basis functions.

The first step in the application of the finite element method is the determination of the variational formulation of the problem. For simplicity, the formulation of the solution will be developed for any particular element e of the domain. Later the solution is extended to all the elements forming the entire domain. The variational form of equation 4.25 over a typical element is obtained by multiplying the equation by a test function v (assumed to be differentiable once with respect to x and y) and integrate over the element domain Ω^e [Reddy, 1984, pp. 196-198].

$$0 = \int_{\Omega^e} \left[\frac{\partial v}{\partial x}\left(T^e \frac{\partial \tilde{h}}{\partial x} \right) + \frac{\partial v}{\partial y}\left(T^e \frac{\partial \tilde{h}}{\partial y} \right) - vf \right] dx\, dy - \oint_{\Gamma^e} v\, T^e \frac{\partial \tilde{h}}{\partial n} ds \qquad (4.29)$$

Where v is the test function, T is the transmissivity in the element, $\tilde{h}$ represents the approximation to the hydraulic head, and the term $T^e \frac{\partial \tilde{h}}{\partial n} ds$ represents the fluxof water across the boundary of the element. This variational formulation indicates that the approxiamtion chosen for the head, $\tilde{h}$, should be at least bilinear in x and y so that the first two terms in Eq. 4.29 and the normal flux term indicated by the line integral are nonzero. If Eq. 4.27 is used to approximate h and Eq. 4.28 is used as linear interpolation functions, the derivative terms in Eq. 4.29 can be expressed as:

$$\frac{\partial \tilde{h}}{\partial x} = \sum_{j=1}^{n} \frac{\partial \psi_j}{\partial x} h_j , \qquad \frac{\partial \tilde{h}}{\partial y} = \sum_{j=1}^{n} \frac{\partial \psi_j}{\partial y} h_j \tag{4.30}$$

Substituting equations 4.30 into 4.29 the equation for an element e becomes:

$$0 = \sum_{j=1}^{n} \left\{ \int_{\Omega^e} \left[\frac{\partial \psi_i}{\partial x} \left(T^e \frac{\partial \psi_j}{\partial x} \right) + \frac{\partial \psi_i}{\partial y} \left(T^e \frac{\partial \psi_j}{\partial y} \right) \right] dx\, dy - \int_{\Omega^e} f\, \psi_i\, dx\, dy - \oint_{\Gamma^e} \psi_i\, T^e \frac{\partial \tilde{h}}{\partial n} ds \right\}$$

$$i = 1, 2, ..., n \tag{4.31}$$

In matrix form equation 4.31 becomes:

$$\sum_{j=1}^{n} K_{ij}^{(e)}\, \tilde{h}_j^{(e)} = F_i^{(e)} \tag{4.32}$$

where:

$$K_{ij}^{(e)} = \int_{\Omega^e} \left(T^{(e)} \frac{\partial \psi_i}{\partial x} \frac{\partial \psi_j}{\partial x} + T^{(e)} \frac{\partial \psi_i}{\partial y} \frac{\partial \psi_j}{\partial y} \right) dx\, dy$$

$$F_i^{(e)} = \int_{\Omega^e} \psi_i\, f_i\, dx\, dy + \oint_{\Gamma^e} \left(T^{(e)} \frac{\partial \tilde{h}}{\partial n} \right) ds$$

$$\tilde{h} = [\tilde{h}_1, \tilde{h}_2, ..., \tilde{h}_n]^T$$

The numerical solution of (4.32) for the head distribution, $\tilde{h}$, requires the exact values of T for element e in addition to the following boundary conditions:

$$\oint_{\Gamma^e}\left(T^e\frac{\partial\tilde{h}}{\partial n}\right)ds \quad \text{on} \quad \Gamma_1^e \qquad \text{Flux boundary}$$

(4.33)

$$H = h_1(x,y) \quad \text{on} \quad \Gamma_2^e \qquad \text{Specified head boundary}$$

The next step towards the solution is the assembly of element equations to obtain the N conditions required for the determination of N nodal values of h over the entire domain. Here, local element nodes are related to global nodes by means of interelement connectivity conditions and local source terms are related to globally specified source terms by means of equlibrium conditions among secondary variables (relationship between the local source or force components and the globally specified source componenets). The next step consists in the assembly of element equations and the global imposition of boundary conditions given by (4.33). Specification of $h = h_1$ (constant head boundary) on some portion Γ_1^e of Γ^e constitutes an essential boundary condition whereas the specification of $T^e\frac{\partial\tilde{h}}{\partial n}ds$ (boundary flux) on some portion Γ_2^e of Γ^e constitutes a natural boundary condition. Here, Γ_1^e and Γ_2^e are disjoint portions whose sum is the total boundary, $\Gamma^e = \Gamma_1^e + \Gamma_2^e$. Finally, the system of equations (4.33) is solved for the nodal values of the head potential, h_i . The area integrals in Eq. 4.32 are numerically evaluated by the Gaussian quadrature method in two dimensions and the solution of the resulting set of algebraic equations is efficiently solved by the Cholesky method. This method takes advantage of the fact that the matrix K is symmetric, positive definite and banded to ease the computational requirements during the solution.

COMPUTATION OF SENSITIVITY COEFFICIENTS

History matching techniques based on the Gauss-Newton method, require the evaluation of the Jacobian J. The elements of this matrix, $J = \partial h_i/\partial b_k$,i = 1,...,M, k = 1,...,p are the sensitivity coefficients, whose significance in the groundwater parameter identification goes beyond simply denoting the derivative of the head with respect of each of the parameters. Analysis of these coefficients, before the identification process begins, can prove vital for the successful convergence of the algorithm. Statistical analysis of the parameters based on this matrix, may also provide valuable information about the reliability of the estimated parameters.

For any identification algorithm involving the matrix A, it must be possible to find its inverse to guarantee a unique solution, this means that det $A \neq 0$. The degree of ill-conditioning of a particular problem is related to the near singularity of matrix A. In an identification problem with n observations and p parameters, J, the Jacobian matrix, is of order pxn and A is of order pxp. Observability of the system also plays an important role in the effects of ill-conditioning of the problem. Depending on the location of the well and the number of data points, it may not be possible to determine uniquely all the parameters from the measurements made at that well. Observability is strictly a function of the aquifer model used. At a given well, pressure measurements may only reflect the values of the parameters in specific zones of the aquifer. If a specific zone away from the well does not reflect the measured head potential, then the system is not observable at that particular location. A more rigorous definition of observability is given by Seinfeld [1969].

Thus, to avoid singularity of A and reduce the ill-conditioning of the problem, there must be at least p nonredundant observations with at least one well located at a point in the aquifer from which the system is observable. If this condition is fulfilled, there will be at least p linearly independent rows among the total of n rows and,

therefore, J will have a rank p. When no redundant information is available (n = p), and one of the rows in J, say, row i, has zero-valued sensitivities $\partial h_i/\partial b_k$ for all k, then the system is not observable from the i-th observation point.

In practice, the number of observation points is limited and usually insufficient with respect to the number of parameters. Furthermore, even if there are numerous observation wells, their location may not be the most adequate to provide information about the system for a well-conditioned matrix A. For these reasons it is important to assess the adequacy of the set of observations for estimating the groundwater parameters before applying the observations to an identification problem.

Sensitivity analysis is the tool used in this study to (1) evaluate the elements of the Jacobian matrix J (also called sensitivity matrix); (2) study the causes of model insensitivity; (3) improve the conditioning of the problem in a least squares sense; and (4) derive reliability estimates of the parameters with the aid of linear statistical methods. The sensitivity coefficients are primarily functions of the particular model, the number and type of parameters, and the boundary conditions. For the case when the aquifer parameters, transmissivity and storativity, vary with space, McElwee [1982] defines the sensitivity coefficients with respect to changes in transmissivity as:

$$U_T(x,t;x_o) = \lim_{\Delta T(x_o)\to 0} \frac{\Delta h(x,t)}{\Delta T(x_o)} \tag{4.34}$$

where Δh is the change in hydraulic head that results when the transmissivity distribution is changed at one point (x_o) by a small amount $\Delta T(x_o)$.

The computation of sensitivity coefficients may be carried out in different ways. In some instances, analytical expressions can be developed to compute the sensitivity coefficients for the case when the parameters do not vary in space.

[McElwee and Yuker, 1978; McElwee, 1980, Cobb, McElwee, and Butt, 1982]. For the case when the parameters vary in space, there are three methods found in the literature: (1) the influence coefficient method, (2) the variational method, and (3) the sensitivity equation method.

The influence coefficient method evaluates the k-th row of the Jacobian matrix J by:

$$\frac{\partial h_i}{\partial T_k} = \frac{h_i(T'+\Delta T_k\, e_k) - h_i(T')}{\Delta T_k} \qquad i = 1, \ldots, n \tag{4.35}$$

Here, ΔT_k is a small perturbation of T_k; e_k is the k-th unit vector; T' is the original parameter vector before being perturbed; h(T') and $h(T'+\Delta T_k e_k)$ are the head distributions before and after the parameters have been disturbed; and n is the number of observations. This method requires perturbing each parameter one at the time. If p is the total number of parameters, (p + 1) forward solutions (evaluations of h) have to be performed at each iteration of the least squares minimization. One major drawback of this approach is that the unknown size of the perturbation ΔT has to be determined by trial and error.

The variational method was introduced by Jaquard and Jain [1965] and has been extensively used in parameter identification ever since [Carter et al., 1974,1982; Neuman,1980; Sun and Yeh, 1985]. This method solves the sensitivity coefficients in a space of reduced dimension $(n_o + 1)$, where n_o is the number of observation wells plus one. The application of the variational techniques to transient problems as [Carter et al., 1974], leads to a system of equations similar to the one found in the forward solution for the heads. This system is solved for an adjoint state variable q(x,y,t). The sensitivity coefficients are obtained following Carter et al. [1974]:

$$\frac{\partial h_l}{\partial T_N^{(i)}} = \iint_{(\Omega_i)} \nabla q'(x,y)\, \nabla h(x,y)\, dx\, dy \qquad (4.36)$$

$$l = 1,2,\ldots,n_0 \qquad i = 1,2,\ldots,N$$

Where n_o is the number of observations; N is the number of nodes in the finite element discretization of Ω; (Ω_i) is the exclusive subdomain of node i; $T_N^{(i)} = T(x,y)$ at node i (i = 1,2,...,N); ∇ is the gradient operator; h(x,y) is the solution of the forward problem for the heads; q'(x,y) is the time derivative of q(x,y); and q(x,y) is the solution of the following problem:

$$\frac{\partial}{\partial x}\left(T\frac{\partial q}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial q}{\partial y}\right)=G_l(x,y)$$

$$\begin{aligned} q(x,y) &= 0 \qquad (x,y) \in (\Omega) \\ q(x,y) &= 0 \qquad (x,y) \in (\Gamma_1) \\ \frac{\partial q}{\partial n}(x,y) &= 0 \qquad (x,y) \in (\Gamma_2) \end{aligned} \qquad (4.37)$$

where

$$\begin{aligned} G_l(x,y) &= 1/P_l \qquad (x,y) \in (\Omega_l) \\ G_l(x,y) &= 0 \qquad \text{otherwise} \end{aligned}$$

P_l is the area of subdomain (Ω_l). The problem (4.37) is called the adjoint problem of the steady state problem (4.25) - (4.26). Since the adjoint equation for q(x,y) has the same form as that of the forward solution, the same numerical scheme can be used to solve for both h and q. By solving the governing equation one time only and solving the adjoint equation for each observation well, all $[\partial h/\partial T_k]$ coefficients can be solved for. Thus, the number of simulation runs at each iteration of the minimization scheme to compute all sensitivity coefficients is $(n_o + 1)$.

The sensitivity equation method treats the sensitivity coefficients as dependent variables in a formal boundary value problem in the same way the heads are treated in the forward solution. The steady state differential equation for the sensitivity coefficients U_T is [McElwee, 1985]:

$$\frac{\partial}{\partial x}\left(T^e \frac{\partial U_T}{\partial x}\right)+\frac{\partial}{\partial y}\left(T^e \frac{\partial U_T}{\partial y}\right)+\frac{\partial}{\partial x}\left(\delta(x-x_o)\,\delta(y-y_o)\frac{\partial h}{\partial x}\right)+$$

$$\frac{\partial}{\partial y}\left(\delta(x-x_o)\,\delta(y-y_o)\frac{\partial h}{\partial y}\right) = 0 \qquad (4.38)$$

where T^e denotes the a constant value of transmissivity in element e; $U_T = U_T(x,y;x_o,y_o)$; x_o and y_o are the coordinates of the perturbation point and δ is the Dirac delta function with the following property:

$$\left.\begin{aligned}\int_{-\infty}^{+\infty} \delta(x-x_o)\,f(x)\,dx = f(x_o)\ ,\ -\infty < x,\ x_o < +\infty \\ \int_{-\infty}^{+\infty} \delta(y-y_o)\,f(y)\,dy = f(y_o)\ ,\ -\infty < y,\ y_o < +\infty\end{aligned}\right\} \qquad (4.39)$$

The application of the finite element method to the solution of (4.38) yields a system of equations almost identical to the one obtained in the forward solution for the heads in Eq. 4.33:

$$K^e\,U_T = F^e \qquad (4.40)$$

where K^e is the same matrix as in equation (4.33), and F^e is now given by:

$$F_i^e = \int_{\Omega^e} \left(\frac{\partial \psi_i}{\partial x} \frac{\partial h}{\partial x} + \frac{\partial \psi_i}{\partial y} \frac{\partial h}{\partial y} \right) dx\, dy - \oint_{\Gamma^e} \frac{\partial U_T}{\partial n} ds \tag{4.41}$$

The two most common types of boundary conditions for the solution of (4.38) are the head specified and the flux specified boundaries. The head specified boundary type is given by:

$$U_T = 0 \quad \text{on } \Gamma_1 \tag{4.42}$$

This is obvious from the fact that $\partial h/\partial T = 0$, assuming that the value of the head remains constant along Γ_1. The second boundary type, flux specified, is defined as:

$$\frac{\partial U_T}{\partial n} = \begin{cases} 0 \quad \text{if } q = \text{constant} \\ \delta(x-x_o)\, \delta(y-y_o) \frac{q}{T^2} \quad \text{if } q = q(x,y);\ x,y \in \Gamma_2 \end{cases} \tag{4.43}$$

where q is the normal flow of water per unit length of boundary Γ_2. In the case of a barrier or impermeable boundary, q = 0.

The sensitivity equation approach to calculate sensitivity coefficients is more convenient than the influence coefficient method since the value of the sensitivity coefficients can be obtained just by solving the system of equations (4.6), once for each parameter at each minimization iteration. This means that we are required to solve the system of equations (p + 1) times at each iteration, which is the same number of solutions as that of the influence coefficient method. However, since the matrix K has already been evaluated for the forward solution of h, these can be stored and used for the solution of (4.6). Only the vector F needs to be calculated for each parameter at each iteration. It is obvious that the variational method is more efficient

if the number of observation wells is less than the number of parameters ($n < p$), which is usually the case in practice. However, the selection of the sensitivity equation approach was made on the basis that this method is more straight forward to implement into the minimization algorithms. Furthermore, the parameterization technique that will be used in this study, is designed to reduce the number of redundant parameters during the minimization. In this case, as the minimization progresses, it is expected that p will be less or equal than n at the final stages of the minimization.

ALGORITHM FOR IDENTIFICATION OF ZONAL TRANSMISSIVITIES

In Chapter 3, an overview of the theory and methods of solution of the nonlinear optimization problem was presented and several numerical artifacts were discussed which may improve the stability of the solution during the optimization process. However, these algorithms alone, cannot cope with the most common problems of the groundwater inverse problems in field applications, namely nonidentifiability and nonuniqueness of the solution. These inherited conditions of the inverse problem stem from the lack of quantity and quality in the head data with respect of the number of parameters that are being identified, near zero head gradient areas, the mathematical function used to represent the parameter filed, and other reasons that were discussed in Chapter 2. In this chapter, a new method is proposed to diminish the effect of these two problems during the optimization process. The technique attempts to reconcile the number of parameters that may be feasibly identifiable with the quantity and quality of informative head data provided for the solution. For least-squares minimization, the maximum number of parameters that may be identified equals the number of observations minus one, however, in practical applications this number may be significantly reduced, if no additional information

about the heads and parameters is provided. The main reasons for this being that the error in the head measurements may exceed several times their standard deviation, high correlation among the parameters and the lack of parameter observability in the head data. The integration of the standard optimization techniques with the proposed methodologies of parameter zonation is illustrated in Figure 1. This flow diagram shows two main groups of operations. In the left side of this flow diagram, from the beginning of the algorithm to the test for convergence in the solution, the operations illustrate the steps in the Marquardt method of optimization with linear constraints on the parameters. The operations in the right-hand side of the diagram are performed to find a more suitable set of parameters of reduced dimension when the Marquardt method fails to find one solution.

Appendix II illustrates the applicability and accuracy of the proposed methods to a groundwater aquifer under flow confined conditions with known analytical solution. This example was carried out to verify the accuarcy of the finite element method to solve for the groundwater steady state forward solution and sensitivity coefficients needed during the nonlinear regression. A simple one-dimensional aquifer with two transmissivity and recharge zones is used in this example. The results from this exercise show the ability of the parameter zonation technique to circumvent instability during the solution and converge to the exact solution. The application of the proposed parameter zonation techinque to a real-life aquifer is presented in Chapter 5 where a solution to the problem of resource management of an aquifer represented by an adequately calibrated model is sought rather than the exact solution to the inverse problem.

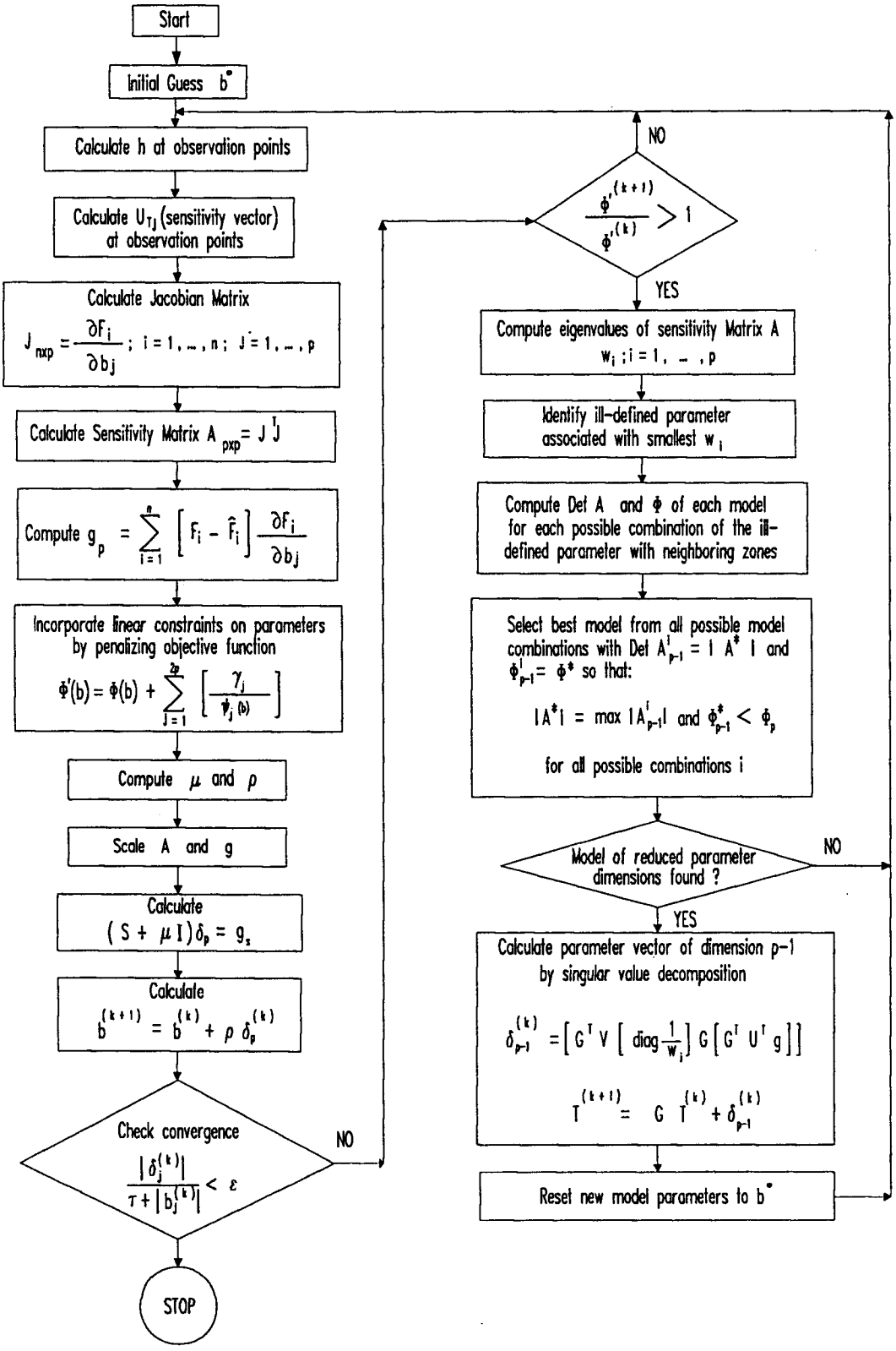

Figure 1. Flow Diagram of Optimization and Parameter Zonation Algorithms

CHAPTER 5

PARAMETER IDENTIFICATION RESULTS

In this chapter, the techniques described in Chapter 4 were applied to examples with hypothetical and field data. The numerical experiments were performed on a confined portion of the Floridan Aquifer located in northwest Florida. The objective of the experiments was to verify the validity and applicability of the proposed methodologies when identifying the transmissivity field over the study area using hypothetical and field data. First, the geologic and hydrogeologic settings of the aquifer are presented in some detail; this explanation is essential to develop an accurate mathematical representation of the physical system. Secondly, the performance of the proposed algorithms was evaluated using head data generated with aquifer parameters, inflows, outflows, and boundary conditions from the literature. Several levels of Gaussian noise were used to corrupt the hypothetical head data. Finally, the transmissivity distribution was identified using field-measured head data and the statistical measures of reliability presented in Chapter 4 were used to analyze the uncertainty of the identified transmissivities.

DESCRIPTION OF STUDY AREA

The aquifer system in the study was the subject of a recent study by Roaza, et al. [1989] to evaluate the extent of ethylene dibromide (EDB) contamination. Most of the monitored water wells were located in an area of approximately 320 square miles in eastern Jackson County, Florida. The study area is bounded on the North by the Alabama-Florida state line, on the South by the interstate highway 90, on the East by Lake Seminole and the Chattahoochee River and on the West by the Chipola River (Figure 2). This region has been the subject of previous studies regarding groundwater

supply and pollution. The hydrogeology and geology of this region have been studied and presented by Moore [1955], Schmidt and Coe [1978], Brooks [1981], Allen [1987], Barksdale [1988], and Wagner [1989]. Most of the geologic and hydrogeologic information presented in the literature is derived from published soil surveys, geophysical logs, driller logs, and pumping test programs.

Geology

The study area lies within the Dougtherty Karst District [Brooks, 1981]. Karst landforms dominate the topography of the region. Dissolution of shallow carbonates is the main process currently modifying the landscape and the low nature of the terrain is a result of stream erosion processes [Moore, 1955]. In this portion of the Floridan Aquifer, terrain elevations range from 70 to 260 feet above sea level. Soils in the area of study have been classified by Duffee et al. [1979] in three main groups as shown in Figure 3. The sand ridge soils located for the most part in the central portion of the study area comprise the Blanton-Troup-Bonifay soil unit. This soil group is generally well to moderately drained and sandy to depths of more than 40 inches and loamy below. This group corresponds to the hydrologic group A with saturated hydraulic conductivities ranging from 0.30 in/hr to 0.45 in/hr. To the east and west of this unit are the uplands soils that are grouped into four soil units: the Fuquay-Chipola-Troup, the Orangeburg-Dothan-Red Bay, the Greenville-Faceville, and the Dothan-Clarendon-Compas soils. These soils are well to poorly drained and may be loamy from depths of 20 inches to 80 inches. These soils fall into the B soil type with saturated hydraulic conductivities of 0.15 in/hr to 0.30 in/hr. The low flatwood soils are located along the west bank of Lake Seminole and the Chattahoochee River. These soils are grouped into the Hornsville-Duplin-Bethera unit. These soils are loamy to clayey with moderate to poor drainage

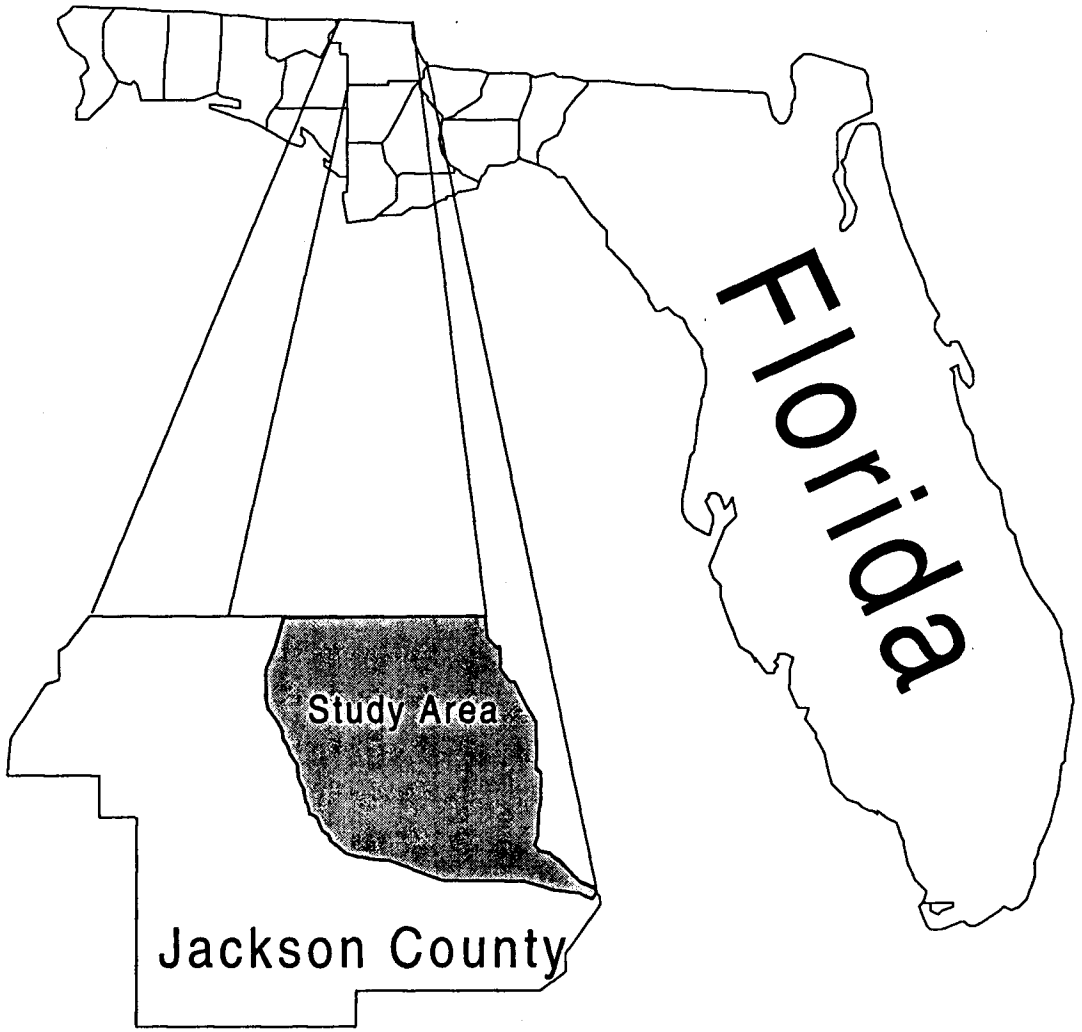

Figure 2. Location of Study Area in Jackson County, Florida

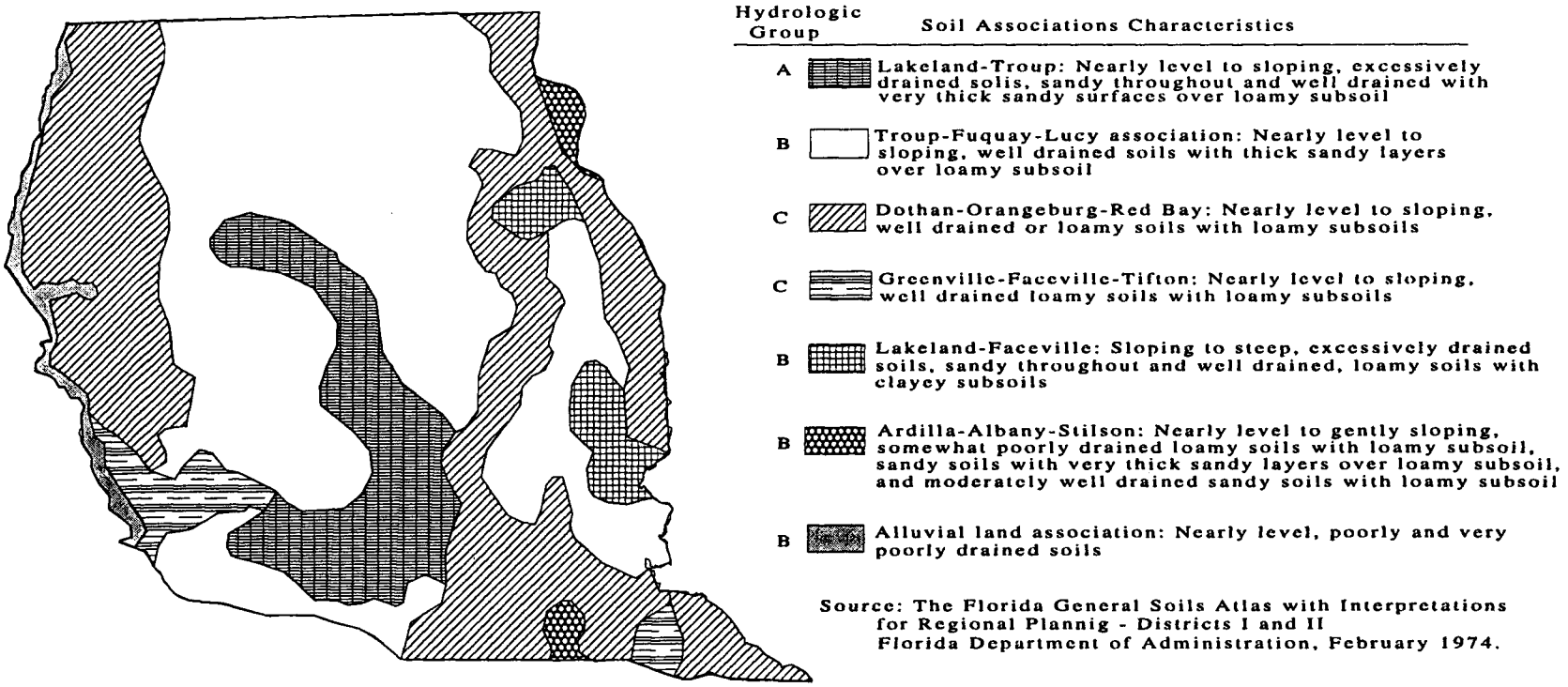

Figure 3. Soil Associations and Their Hydrologic Group Classification

capacity. These are C hydrologic type soils with saturated hydraulic conductivities ranging from 0.05 in/hr to 0.15 in/hr.

The principal source of potable and irrigation water in north Florida is the Floridan Aquifer. This hydrogeologic unit comprises three Tertiary age marine carbonate units. The carbonate rocks of the Floridan Aquifer are highly fossiliferous and consist mainly of limestones, dolomitic limestones, dolomites and marl. In the northern half of the study area, the Floridan Aquifer consists of solely the Ocala Limestone. In the southern half, the aquifer incorporates the Ocala and two stratigraphically higher units, the Marianna Limestone and the Suwannee Limestone. Regionally, the structural top of the aquifer dips and the aquifer thickens to the South. The top of the aquifer is highly irregular because of buried and surficial karst features. The thickness of the Floridan Aquifer in the study area ranges from 100 to 250 feet. The thinnest section is located in the northern part of the study area. The aquifer thickens to the South where it is less than 150 feet thick in areas where the Ocala Limestone and the Suwannee limestone solely comprise the aquifer.

Below the surficial soil layers, there is a thin layer of unconsolidated clastic sediments. These sediments, with the top soil layer, comprise an overburden which overlies the carbonates of the Floridan. These overburden materials are described as a post-Miocene terrace and river flood plain residuum deposited by stream erosion and deposition [Moore, 1955]. The composition of these materials includes sand, sandy clay, clayey/silty sand, and clay. The thickness of the overburden in the study area ranges from 14 to 89 feet with a median of 45 feet and a mean thickness of 49 feet.

Because the carbonate rocks of the Floridan are highly soluble in water, the development of karst features is common. Among such karst features are enlarged joints and fractures, sink holes, caves, and solution bracias. Secondary porosity develops as the dissolution process acts on the carbonate rock of the aquifer. Conduit flow is evident in

many parts of the aquifer where recent drilling programs have encountered numerous solution cavities as much as five feet in height. This secondary porosity can be seen at the Florida Caverns State Park where the unsaturated portion of the Ocala Limestone is riddled with solution cavities. Some of these conduits are large enough to walk through.

The carbonate rock solution activity is reflected in the surface of the terrain as sinkholes. The study area has a high average sinkhole density of about eight identifiable sinkholes per square mile. Other karst features of relevance in the area are paleosinks or buried sinkholes that are not identifiable by conventional photogrametric or topographic methods. Although lithology logs of a few wells drilled into these features are available, the distribution of paleosinks throughout the study area is unknown.

Precipitation

Several long term hourly precipitation records (1938 to 1988) near the study area, indicate that the mean annual precipitation is between 51.4 and 56.6 inches. The annual rainfall distribution in the study area is typical of the northwestern Gulf Coast with dominant frontal activity in the months of January, February and March. This rainfall activity is characterized by widespread and uniformly distributed rainfall over large portions of the study area. Rainfall events are characterized by long duration and low intensity. The months of June, July, August and September are the wettest months. These months account for over 40 percent of the total annual precipitation in the region. Rainfall events are usually associated with convective evening thunderstorms of short duration, high intensity, which are unevenly distributed over the study area. The driest months of the year are typically October and November with several occurrences of zero monthly precipitation for these months in the 50-year record period.

Surface Water

Most of the surface runoff generated by precipitation over the study area is lost back to the atmosphere as evapotranspiration or reaches the aquifer formation by infiltration. This groundwater is drained out of the study area as baseflow into the Chipola River, Lake Seminole, and the Chattahoochee River. Figure 4 illustrates the main surface water drainage features found in the study area. Clearly, no significant surface drainage features can be found in the area other than the Blue Spring near Marianna and many other springs along the Chipola River. All these springs are karst features that represent a major outlet for groundwater discharge into the Chipola River. Scattered instantaneous discharge measurements at the spring were used to determine a mean discharge of 190 cfs for Blue Spring [Rosenau et al., 1977]. This flow represents almost half the total groundwater discharge of the Chipola River near Marianna below Blue Springs. The average baseflow discharge on the Chipola River above Blue Springs has been estimated at 225 cfs. Several other springs in the western edge of the study area also discharge groundwater from the Floridan Aquifer into the Chipola River. Among them are Bosel Spring and Hayes Spring with estimated average baseflow discharge of 73 cfs and 18 cfs respectively.

Areal Aquifer Recharge

Quantification of areal discharge to the Floridan Aquifer in the study area is a difficult task. Water budget methods based on precipitation and evapotranspiration data are not accurate due to the limitations of long term hydrologic data, specifically evapotranspiration data. The study area would be particularly well suited for this kind of recharge estimation since there are practically no surface water drainage features in the area (Figure 4). This means that the majority of the rainfall which falls over the study

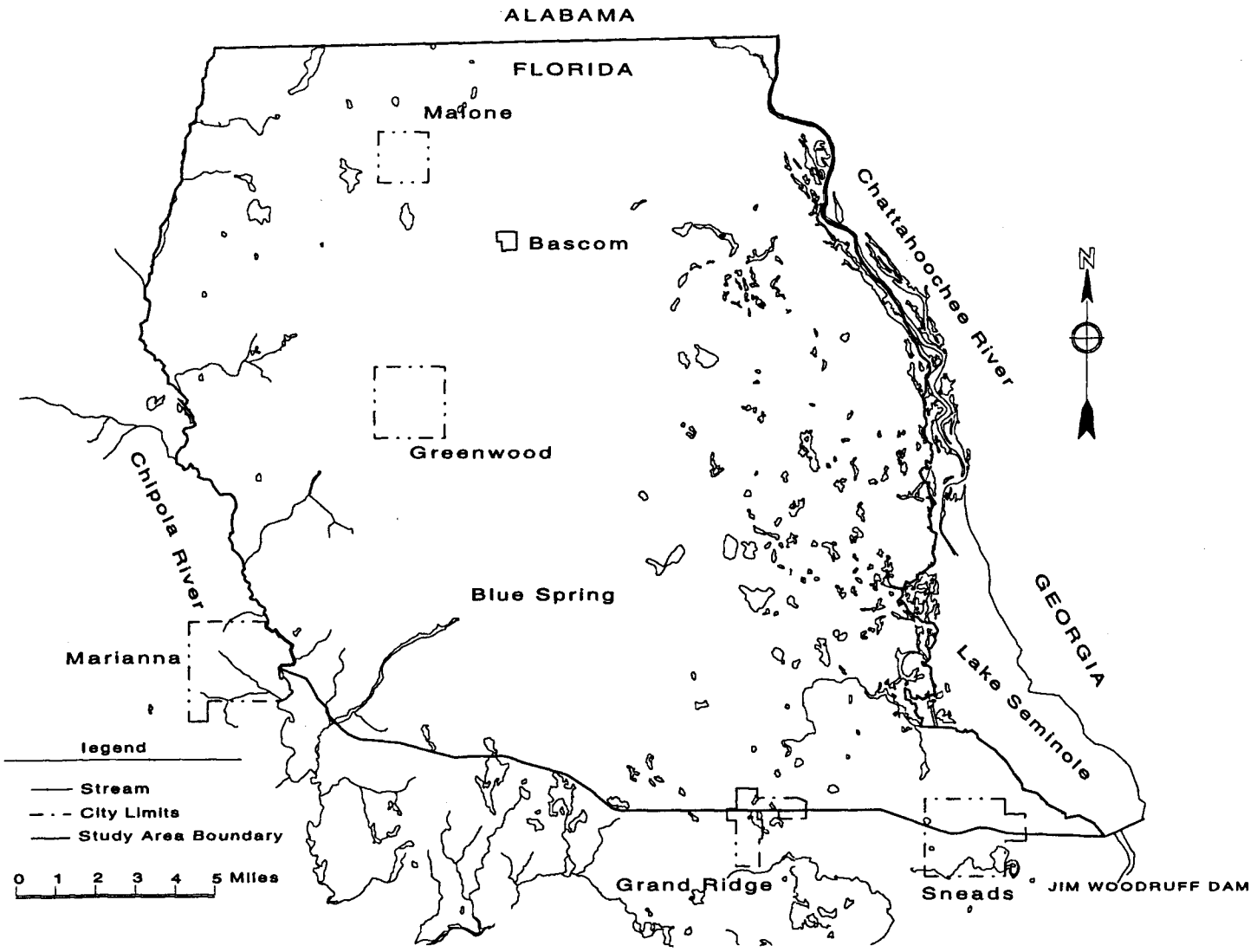

Figure 4. Surface Water Features in Study Area

area is drained out as base flow or lost back into the atmosphere as evapotranspiration. Unfortunately, there are no adequate evapotranspiration data available in the region.

Alternative methods based on geologic and soil characteristics can sometimes be used to evaluate recharge potential. These methods require knowledge of variables such as hydraulic properties of the soils; vegetative cover; permeability and thickness of the confining unit; density and clustering of surface karst features; the thickness of the sediment overlying the aquifer; relative position of the aquifer to land surface and the position of the surficial aquifer in relation to the potentiometric surface of the Floridan Aquifer. Although maps of potential recharge can be developed when this information is available, the actual filed response between recharge, these parameters and precipitation needs to be established through field measurements. Lack of information prevented the application of this approach to estimate the areal discharge distribution over the study area.

An alternative method to estimate average recharge to the Floridan Aquifer in the study area is by evaluating long-term stream flow records. Assuming that (1) there is a long term quasi-steady state equilibrium between recharge to the Floridan Aquifer and surface discharge, (2) there is no significant pumping or other diversions, and (3) ignoring short-term variations in the amount of water in storage, then recharge equals discharge.

Areal recharge into the study area were estimated by evaluating long-term stream flow records during low flow periods. It is well known that the Chipola River receives most of its base flow from the Floridan Aquifer. There are many springs along its length in Jackson County from which the most notorious is the Blue Spring. This spring has an estimated average discharge of 100 million gallons per day [Rosenau, et at., 1977].

Base flow estimates were computed using flow records in the Chipola River by neglecting any significant pumping and other diversions. Daily flow averages from 1943 to present are available for a U.S. Geological Survey flow gauge near the city of Altha.

The contributing area for this gauge is approximately 781 square miles. The average discharge for 53 years of record (1935 to 1988) is 1,495 cfs or 26 inches per year. Low flow estimates were computed by using daily streamflow data for the month of October in the period from 1960 to 1988. In 14 of 28 years (1961-1988) the mean monthly discharge was lowest in either October or November with almost no difference between the October and November mean monthly discharge. From this analysis, base flow was estimated to range between seven and fifteen inches per year [Roaza et al., 1989]. For comparison, the two-year, seven-day continuous low flow at the Altha flow gauge is about 550 cfs (9.6 inches per year). The ten-year, seven-day low flow is about 400 cfs (6.98 in/yr) [Maristany et al., 1984]. Using streamflow information at the U.S. Geological Survey flow gauge near Altha, Florida, a value of 600 cfs (17.52 in/yr) of areal aquifer recharge was established for the calibration period described in the next section. This higher value of base flow, which differs from the long-term low flow value range between 7 and 10 inches per year, was assigned to the "wet" season in the month of July, 1989.

Potentiometric Head Data

Because of the spatial variability of the overburden thickness and the variations in the elevation of the top of the carbonate sequence, the groundwater flows under both confined and unconfined conditions in the Floridan Aquifer. Unconfined flow occurs wherever the potentiometric surface is located below the top of the limestone, whereas confined flow can be found where the potentiometric surface is above the top of the limestone.

Potentiometric data in the study area were obtained from a variety of sources and were measured in a variety of ways. A regional potentiometric map was developed by the U.S.G.S. based on a finite difference computer model [Bush and Jonhston, 1988]. This steady state potentiometric map was computed based on regional values of recharge,

leakance, pumpage, and block transmissivities. More recently, Wagner [1989] developed a potentiometric surface map of the Floridan aquifer system in the panhandle area (Figure 5) based on a regional database of potentiometric data. General inferences and descriptions of the flow field can be derived from the potentiometric map in Figure 5. Major sources of groundwater in the Floridan aquifer include areas of high recharge in the central portion of the study area. Hydraulic gradients generally are steepest close to areas of high recharge and tend to become much shallower downgradient. This pattern may suggest an interaction of several factors such as flow divergence, vertical leakage, discharge from springs, and drastic changes in permeability. Areas of high hydraulic head include the northern and southern portions of the study area and a ridge of high head that runs down the center of this area. Discharge areas include the length of the Chipola River and the Blue Spring in the West and Lake Seminole and the Chattahoochee River in the East. All these discharge features are in direct hydraulic connection with the Floridan Aquifer. The Blue Spring, for example, with a mean discharge of about 100 cfs, is well known to have a significant impact on the potentiometric surface over a large portion of the study area.

Most of the published potentiometric data in the study area are from water wells or oil exploration wells. Because any regression procedure used for parameter identification depends on the amount and reliability of the observed head data, it is particularly important to collect and use the most accurate head data.

Due to the lack of potentiometric data in the study area, a sampling program was carried out to measure the potentiometric surface of the Floridan Aquifer in the region [Roaza et al., 1989]. The sampling program conducted two measurements to determine the relative differences in the elevation of this surface between the "wet" and the "dry" seasons. In a typical year and outside the influence of significant pumping, water levels in the Floridan Aquifer are generally lowest in October, November and December. Areal

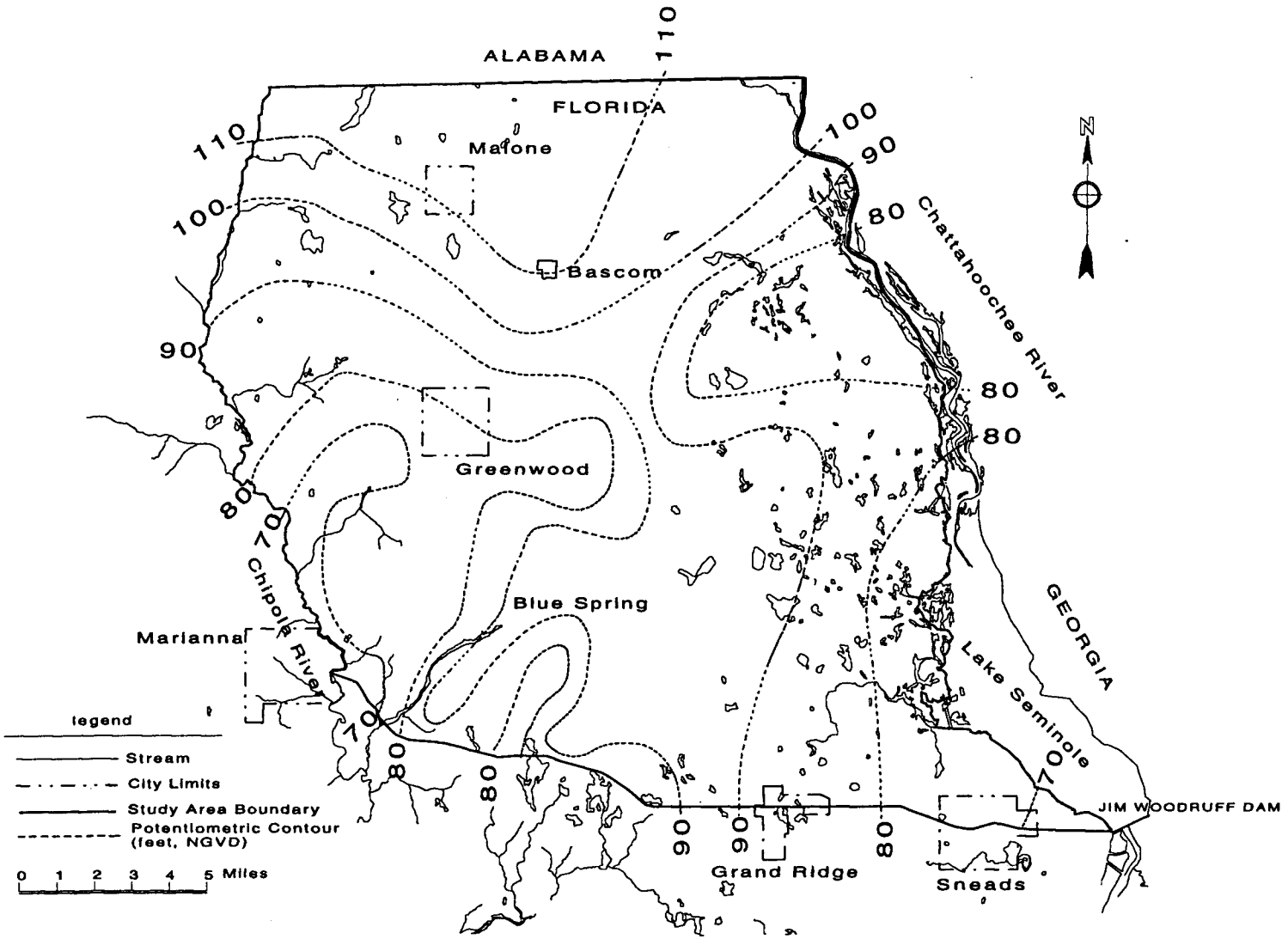

Figure 5. Contour Map of the Potentiometric Surface of the Floridan Aquifer Over the Study Area, May 1986

recharge diminishes during this part of the year when the of lowest precipitation occurs. Significant rainfall and reduced evapotranspiration losses during winter months result in higher recharge and correspondingly higher water levels in the months of April and May. The "dry" period sampling was carried out between October 31 and November 4, 1988. Water levels were measured at a total of 84 wells. All water level measurements were made with a chalked steel tape graduated in 0.01 foot increments. The second set of water level measurements was made between July 5 and 11, 1989. Head measurements were made at a total of 96 wells, including 77 of the wells that were measured in October and November 1988. In addition, there were several wells with long term water level records. The most complete record correspond to the Hollingsworth well near Malone with a continuous record dating back from 1986. During the "dry" period sampling, water levels steadily declined to normal low levels. However during this period, a total of 25.8 inches of rain was recorded at Greenwood, Florida. This is about half the mean annual precipitation for the region. A significant rise in water levels (5 to 10 feet in the northwest portion of the study area) took place in the region as a result of these rains. Figure 6 illustrates the potentiometric surface for the Floridan Aquifer during the "dry" (October-November) and "wet" (May-July) seasons. The groundwater flow patterns derived from the data for the wet and dry seasons show some common characteristics. Water in the Floridan Aquifer is observed moving from areas of high hydraulic head to the principal discharge areas. Areas of high hydraulic head include the northern and southern portions of the study area and a ridge that runs down the center of the region. The discharge areas include the Chipola River and Blue Spring in the West and Lake Seminole and the Chatahoochee River in the East. All these discharge features are in direct hydraulic connection with the Floridan Aquifer.

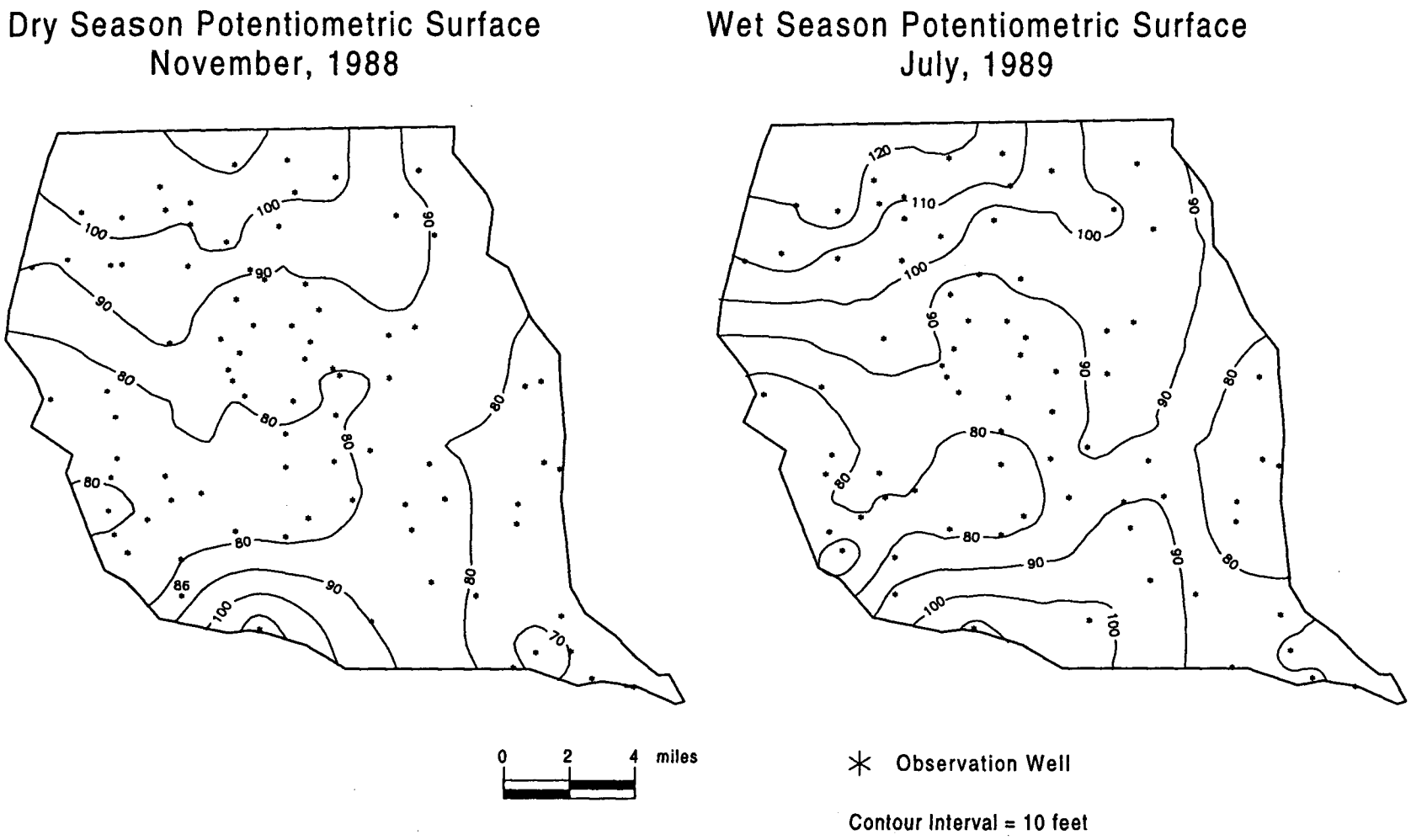

Figure 6. Potentiometric Surface of the Floridan Aquifer During "Dry" and "Wet" Sampling Seasons

Aquifer Parameters

The regional hydraulic properties of the Floridan in the study area are generally unknown. Aquifer parameter information is very limited and consists of isolated pumping test data and scattered specific capacity data at a few locations throughout the study area. Specific capacity is the discharge of the well divided by the associated drawdown and is usually expressed in units of gallons per minute per foot of drawdown (gpm/ft). Figure 7 illustrates the location of the wells with specific capacity data in the study area. Specific capacity may be used to estimate aquifer transmissivity. Lowman [1979] provides a version of the Theis equation that may be used to estimate transmissivity from specific capacity data, subject to a number of assumptions. Records of a total of 15 specific capacity tests were located for this study. All these data were provided by well drillers. Using Lowman's equation with the available specific capacity data in the study area, the estimated values of the transmissivity in the Floridan range between 1,000 and 50,000 ft^2/day. Aquifer test data from a multi-well aquifer test is also available [Wagner, 1980]. The test was conducted four miles northeast of Marianna and had a duration of 72 hours. The computed transmissivity from this test was 50,000 ft^2/day and the storage coefficient was calculated as 0.0003. All this scattered information about the aquifer properties is subject to large uncertainties and cannot be used to describe regional aquifer properties. However, a range of parameter values can be obtained that may be useful in an inverse modeling exercise when selecting initial estimates and the range of values for the regional parameters. Roaza et al. [1989] assigned zonal transmissivities for the study area based on trial-and-error calibration for the transmissivity distribution. The initial size and shape of each zone were estimated from existing information about the hydrogeologic makeup of the region. The spatial variability of the calibrated transmissivities is shown in Figure 8. This map shows an area of low transmissivity along the northern edge of the study area. This corresponds to

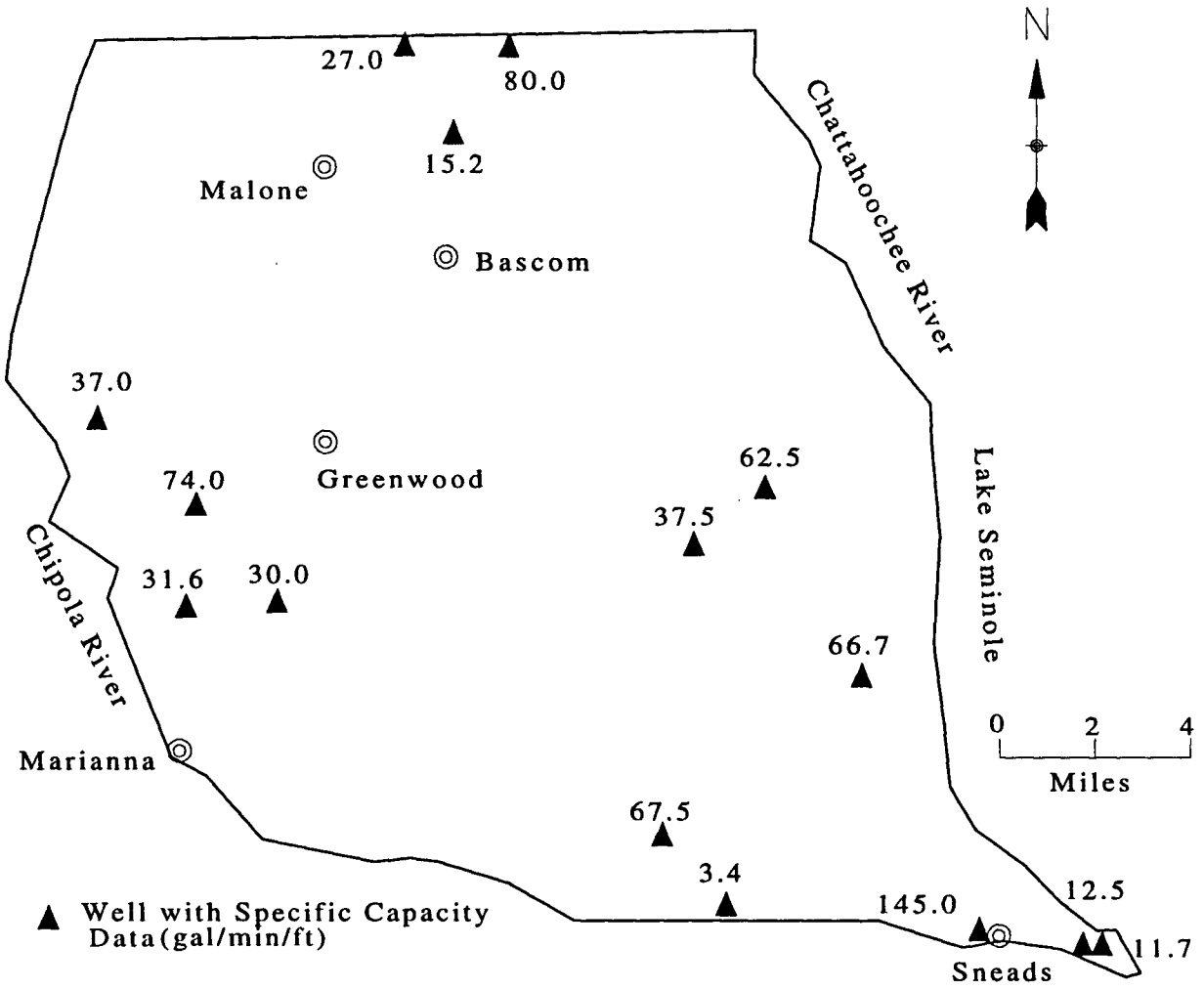

Figure 7. Location of Wells with Specific Capacity Data

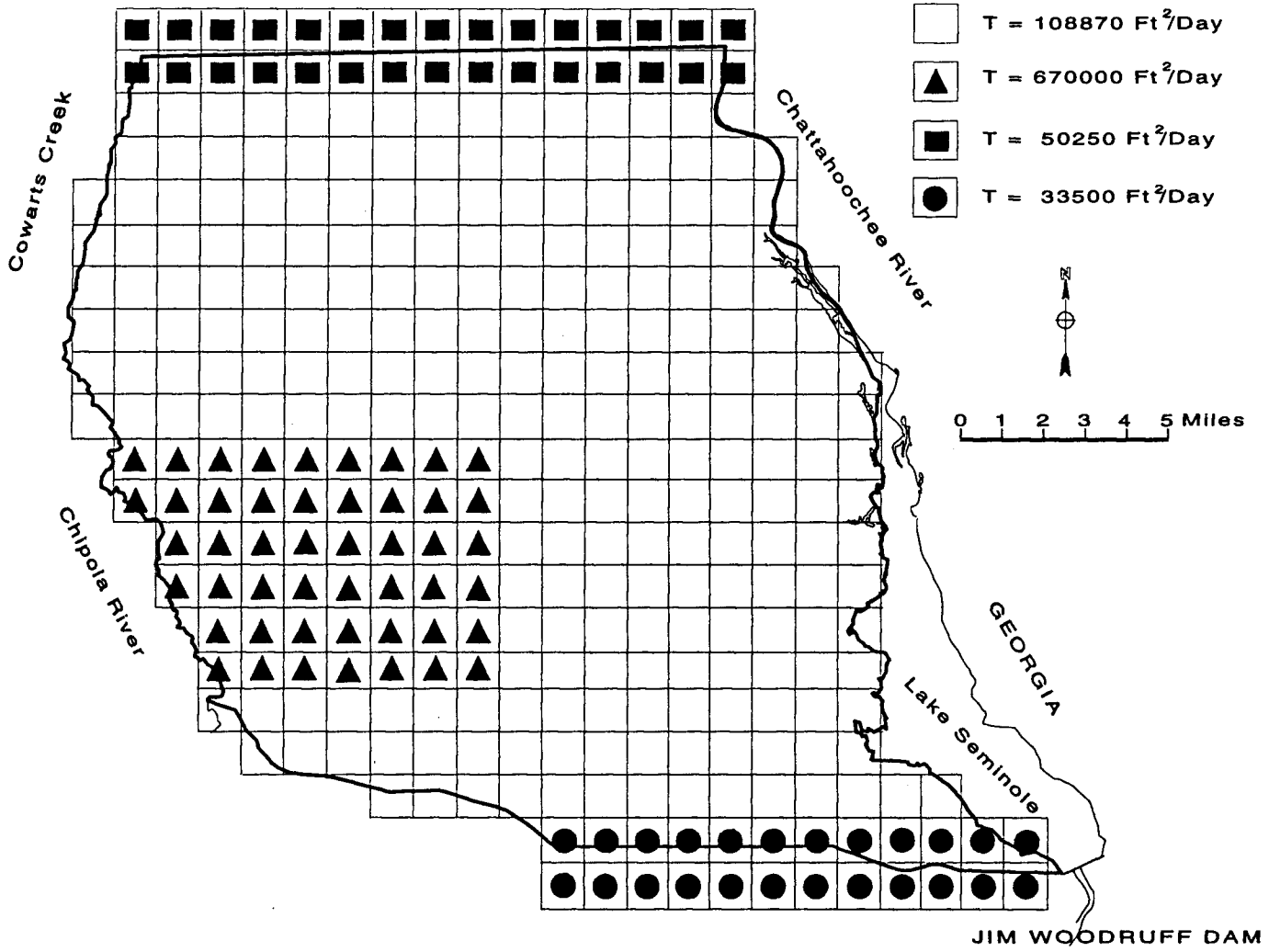

Figure 8. Calibrated Transmissivity Distribution in Study Area (Roaza, 1989)

the area where the aquifer is thinnest. An area of high transmissivity was identified near Blue Spring. The existence of such an area was inferred from the potentiometric head distribution in this area. Similarly, an area of low transmissivity was inferred for the southern edge of the study area.

NUMERICAL MODELING

The principal task of this study was the development, verification, and application of numerical techniques to identify regional groundwater parameters based on noisy potentiometric field data. Of special interest in this study were the effects of corrupted field data and lack of information regarding both the head distribution and the aquifer parameters in the study area. The numerical techniques described in Chapter 4 were applied to the identification of zonal transmissivities in two stages. In stage one, the ability of the algorithms to identify the transmissivity distribution based on hypothetical noiseless head data was investigated. For this purpose it is necessary to have an "exact" head distribution that can be corrupted with noise and then used to identify the transmissivities. The identification of transmissivities using noiseless data, although an academic exercise, may give some insight into the model's performance under optimum conditions. Then by applying white noise of predetermined mean and variance to the data, one could evaluate the propagation of uncertainty of the estimates due to error in the head data. In stage two, a set of actual field head data was employed to identify the zonal aquifer transmissivities.

Preliminary Forward Solution

Groundwater flow throughout the portion of the Floridan aquifer corresponding to the model domain was assumed to be governed by the two-dimensional steady state, Equation 4.1. This equation represents a model for a medium that is behaving as if it

were isotropic and porous. Thus it is assumed that the localized secondary permeability features can be neglected as distinct properties at the regional scale at which the aquifer system is being analyzed.

In this model, the variability of the transmissivity T was represented by subdividing the aquifer into several zones. The shape and size of these zones were determined using hydrogeologic information of the aquifer in the study area. The zonation of transmissivity values is necessary because sufficient information is never available to estimate the transmissivity distribution (T) as a continuously varying function of space. Aquifer parameter zoning allows a single value of T to be estimated for each of several predefined zones. The number of zones for which T can be estimated depends on the amount of detail known about the aquifer characteristics and on the characteristics themselves. It is well known that the discontinuities of T usually do not create large irregularities in the hydraulic head distribution during the forward solution because of insensitivity of the heads to T. Thus, the transmissivity field in the Floridan Aquifer corresponding to the study area was characterized using the zonation method. In this study, 49 8-node quadrilateral finite elements were used to characterize the transmissivity field over the study area. The initial number of transmissivity zones was limited to 37 which is less than the number of observation wells (49). This precaution was taken since a regression procedure will be employed in the next section to identify the parameters. In regression procedures, it is desirable to have a much larger number of observations than unknown parameters.

For computational simplicity, model nodes were located to coincide with observation wells, springs and hydraulic and geologic boundaries. The 49-element discretized domain totaled 128 nodes and it is shown in Figure 9. The location of the observation wells is shown in Figure 10.

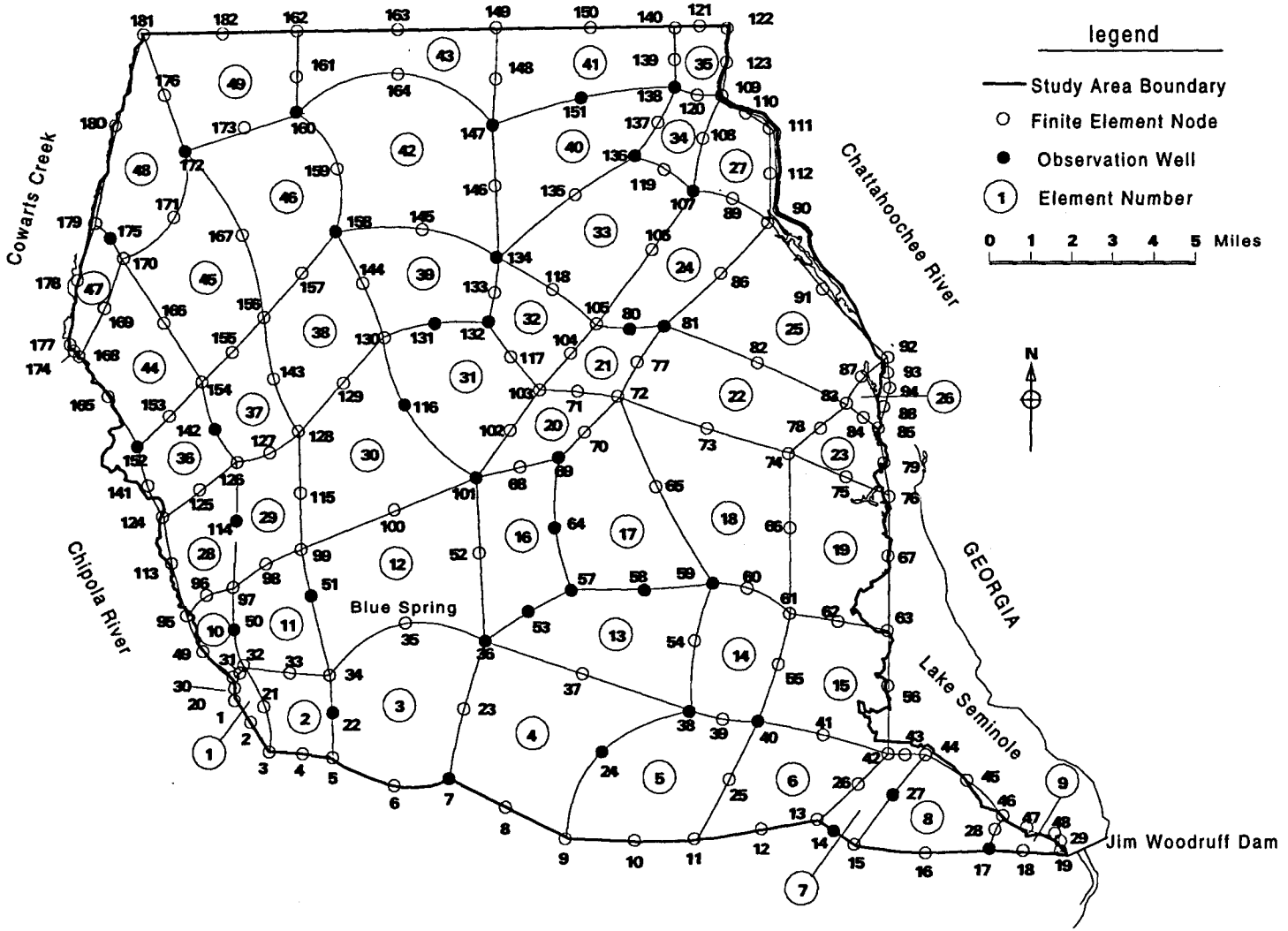

Figure 9. Finite Element Discretization of the Portion of the Floridan Aquifer Corresponding to the Study Area

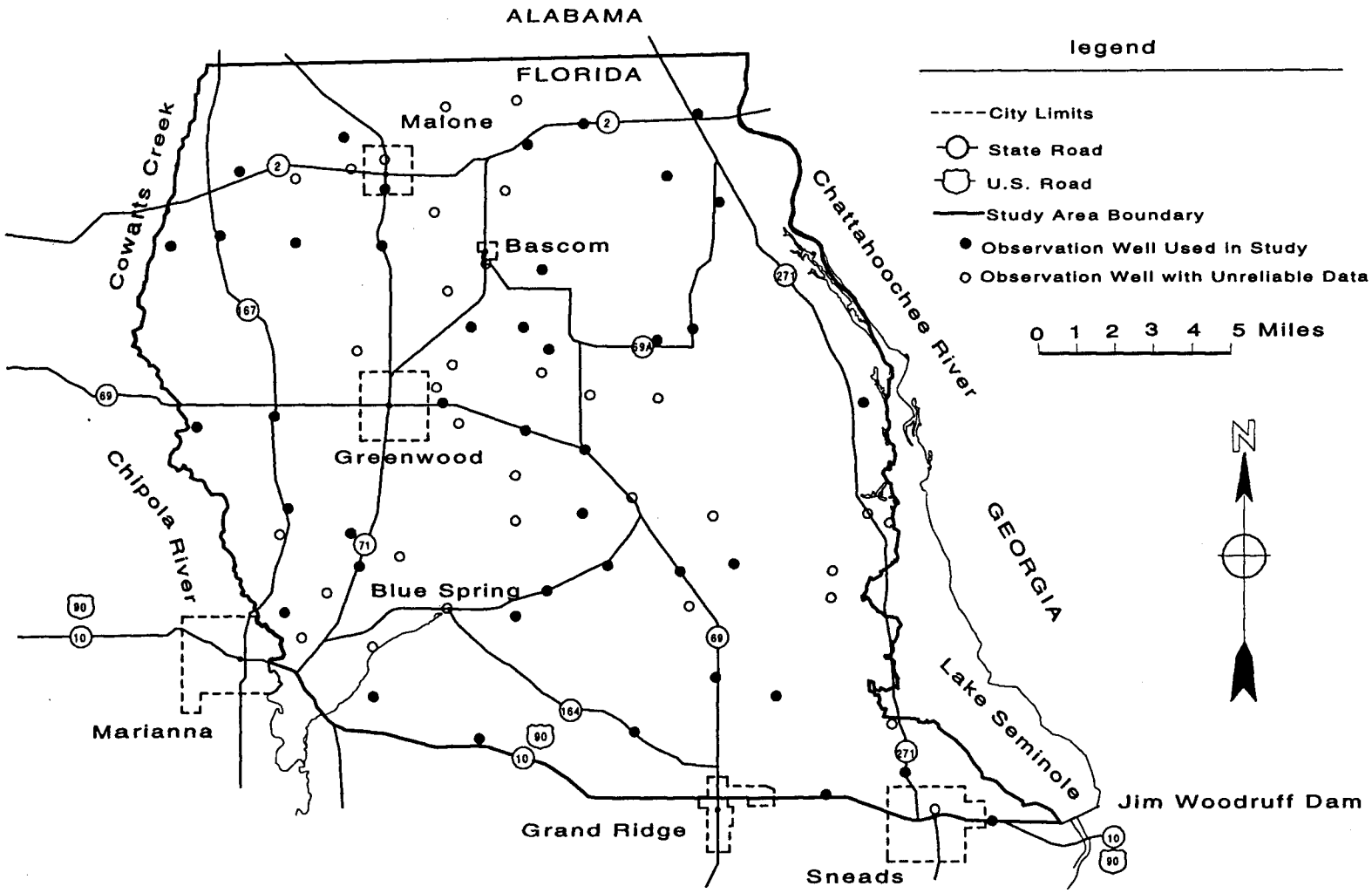

Figure 10. Location of Observation Wells in Study Area

Two types of boundary conditions were employed in this modeling effort. A specified head boundary is used on the eastern edge of the model domain to simulate the effect of the Chattahoochee River and Lake Seminole. For the domain boundary corresponding to the Chattahoochee River the head varies linearly north to south from a value of 80 to 77 feet. The variation of head values along the river was computed using the slope of the bottom of the channel. Head values corresponding to Lake Seminole were assigned a constant value of 77 feet, which is the approximate mean elevation of the lake during the time when the well data was collected. No-flow boundaries are used on portions of the northern, western and southern boundaries. A no-flow boundary is used on the northern edge, because the carbonates that comprise the Floridan aquifer pinch out in southeast Alabama, just north of the study area. The assignment of no-flow boundaries on portions of the southern and western edges was guided by the behavior of the potentiometric surface of the Floridan Aquifer in these areas mapped in previous studies [Wagner, 1989]. The western boundary corresponding to the Chipola River was represented in the model as a flow boundary In this study, it is assumed that the observed head distribution represents an average steady state flow condition in equilibrium with present withdrawals, therefore, this model only includes those withdrawal rates that represent major long-term stresses on the aquifer and for which the discharge rate is fairly reliable. Thus, by using the long term base flow records for the Chipola River, a discharge value of 62.7 cfs was assigned along this boundary. The discharge was assigned to nodes corresponding to the element nodes on this boundary segment. The northern portion of this boundary segment was assigned a larger discharge because of the convergence of flow lines in this area inferred from available potentiometric maps. The effect of Blue Spring was simulated as a point discharge with a value of 208 cfs. This discharge was estimated from historical discharge data taken at the spring.

The steady state model calibration was performed using the "wet" season head data set. It is obvious that this set of data is more suitable for inversion than the "dry" season data because of the larger hydraulic gradients throughout the study area. During this period, the areal recharge over the study area was estimated at 600 cfs which corresponds to 17.52 inches per year. In this study, no attempt was made to estimate the spatial distribution of areal recharge which can be incorporated as part of the unknown aquifer parameters to be identified. The areal recharge was modeled as being uniformly distributed over the study area.

Given all these hydrogeologic elements, the steady state distribution of the potentiometric head was computed as a function of the aquifer parameters, the inflows, and the outflows. The resulting head distribution is presented in Figure 11. This head distribution was necessary to fit exact and white-noise corrupted head data with the proposed regression model.

Inversion of Error-Free Data

The first numerical inverse experiment considered, was the inversion of a hypothetical data set of head measurements assumed to be free of error. This data set of heads represents an unlikely scenario from the practical point of view, but it is useful to verify the performance of the proposed methodologies under ideal conditions, before considering more realistic scenarios. The initial and final parameters and their estimated standard errors for the 37-parameter case are shown in Table 1. All the identified transmissivities show large standard errors, in some cases as large as 1246 percent of the value of the identified transmissivity for T in zone 1. This example clearly represents an ill-conditioned problem in which the statistical uncertainty of the identified parameters overwhelms the parameter structure uncertainty. The large variances encountered in Table 1 are due to lack of information provided by the given head values to properly

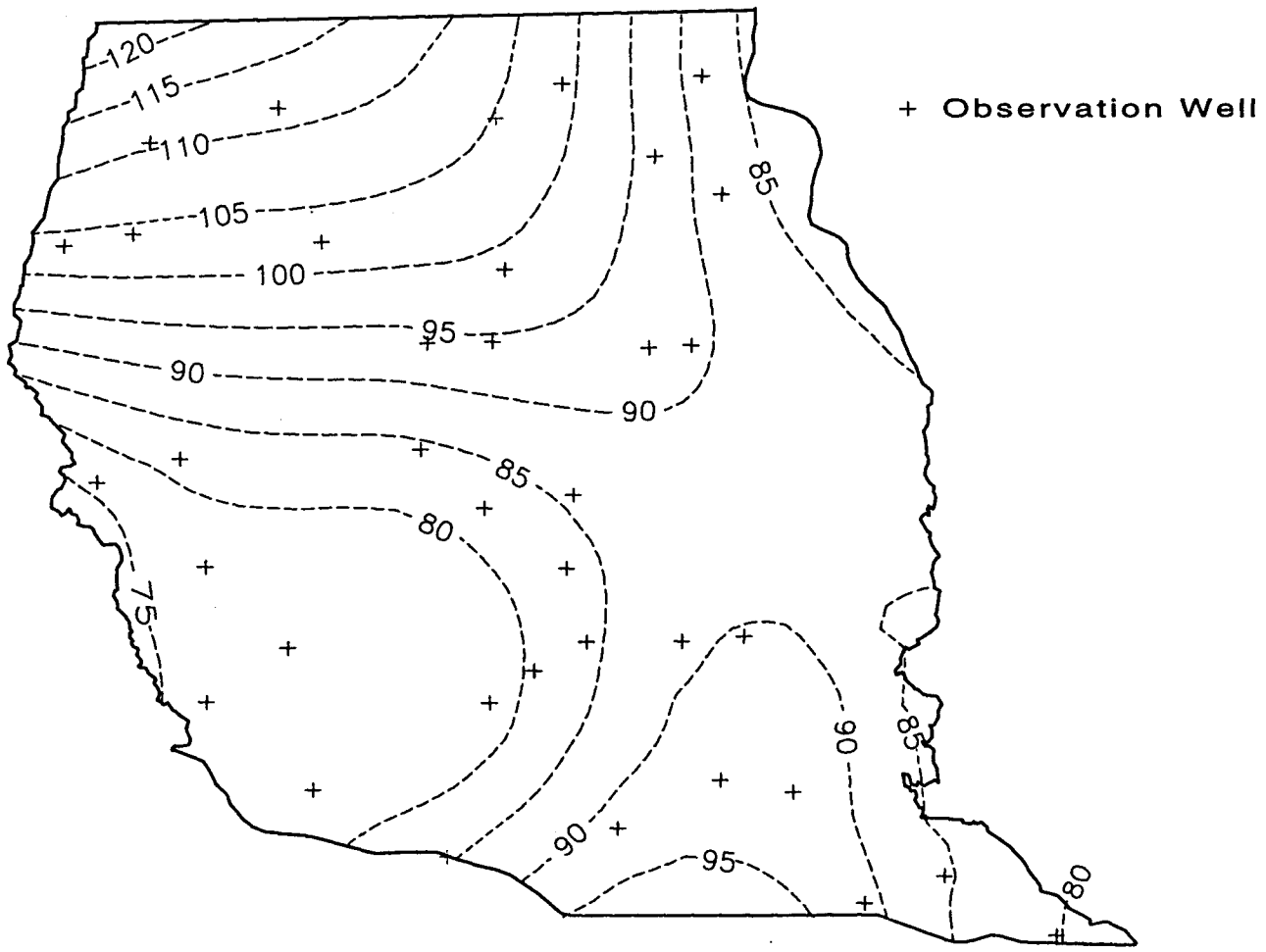

Figure 11. Head Potential Contour Map from Forward Solution Using "Trial-and-Error" Calibrated Transmissivity Distribution

identify all the parameters simultaneously. There are two common methods in the literature to solve this problem. The easiest approach is to incorporate prior information about the ill-defined parameters or eliminate them completely from the regression by obtaining their value in the field. This approach may not be feasible for practical and economical reasons. The second approach involves the use of sensitivity analysis to establish appropriate locations of observation wells throughout the aquifer which may incorporate the necessary information about the sought parameters into the regression. This is a separate class of experiment design problems and will not be further elaborated in this study. Instead, a third approach has been used in this study in which the ill-defined parameters are eliminated from the regression by combining transmissivity zones in such a way that the overall sensitivity of the system is increased to a level in which a feasible set of transmissivities can be identified. The feasibility range for all transmissivity parameters was established from field data about the parameters and was incorporated into the regression in the form of parameter constraints.

The first set of identified transmissivities showed several ill-defined parameters as indicated by the large variances in Table 1. As described in Chapter 4, the parameter with the current largest variance is eliminated from the regression if there exists a combination of zones which not only increase the sensitivity of the system but also keep the value of the objective function Φ close to the sought minimum. This technique is applied until convergence of the solution is achieved according to the convergence criteria. The aquifer was initially subdivided into 37 transmissivity zones. Figure 12 shows the initial transmissivity distribution with 37 transmissivity zones. Notice that a large transmissivity zone was designated on the eastern portion of the study area. The reason for this is the lack of head data in this area and any attempts to identify multiple zones with no informative head data may lead to ill-defined parameters.

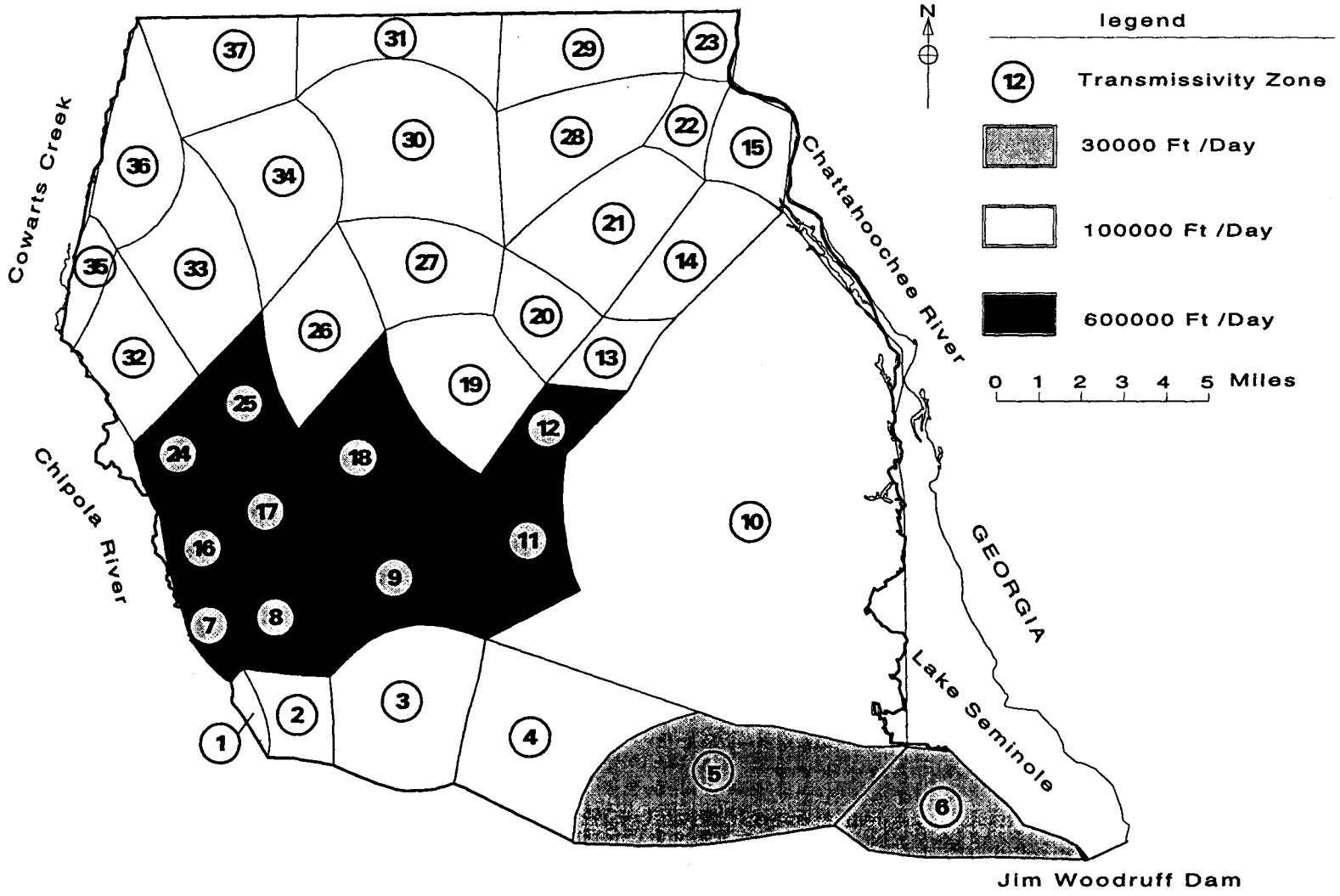

Figure 12. Initial Transmissivity Distribution for Regression Model with 37 Transmissivity Zones

Table 1
Initial, Final, True Value and Variance of T for 37 Zone Aquifer

Zone	Initial Value of T (ft^2/day)	Final Value of T (ft^2/day)	Exact Value of T (ft^2/day)	Variance
1	100000	310097.03	108870	3.8642E+06
2	100000	101272.08	108870	1.0573E+05
3	100000	109873.51	108870	1.4170E+04
4	100000	108884.55	108870	3.5578E+03
5	30000	33300.87	33500	2.6472E+03
6	30000	33256.58	33500	1.3714E+03
7	600000	566901.93	670000	3.3557E+06
8	600000	646918.18	670000	5.3926E+05
9	600000	682470.62	670000	2.4790E+05
10	100000	108860.78	108870	1.7299E+03
11	600000	657348.43	670000	1.4234E+05
12	600000	670206.87	670000	6.7468E+05
13	100000	113158.28	108870	1.4083E+05
14	100000	106794.01	108870	1.0028E+05
15	100000	114680.08	108870	1.2200E+05
16	600000	623077.00	670000	2.2368E+06
17	600000	656508.06	670000	6.8143E+05
18	600000	670737.93	670000	3.1946E+05
19	100000	113080.12	108870	1.4144E+05
20	100000	104946.70	108870	1.8166E+05
21	100000	113551.10	108870	1.8439E+05
22	100000	116757.42	108870	1.6733E+05
23	100000	101408.23	108870	8.4310E+04
24	600000	671712.25	670000	4.9319E+05
25	600000	595309.93	670000	2.5305E+06
26	100000	97981.91	108870	2.8277E+05
27	100000	116440.89	108870	2.6252E+05
28	100000	119706.30	108870	1.0566E+05
29	100000	91734.66	108870	1.7849E+05
30	100000	111986.35	108870	3.2586E+05
31	100000	151909.62	108870	7.5703E+05
32	100000	104574.09	108870	3.7911E+05
33	100000	123926.66	108870	2.6396E+05
34	100000	89644.09	108870	3.6375E+05
35	100000	123966.85	108870	8.4360E+05
36	100000	124987.98	108870	3.0562E+05
37	100000	390812.25	108870	3.6783E+06

Optimization of the parameter values was carried out without reaching convergence of the solution after the number of iterations reached the allowed maximum of 200. The residual error of heads in this example was small but not as small as expected in a case where noiseless data are being fitted. The value of the objective function for the 37-zone model was reduced from an initial value of 7.0053 to a final value of 0.02676 after 100 iterations. Close examination of the value of the parameters during the minimization process indicated that not all the parameters converge to their true values. The largest parameter standard errors were associated with zones 1, 7, 16, 25 and 37 respectively, indicating that these parameters are ill-defined when all 37 parameters are identified simultaneously using the given head data. For the initial model with 37 parameters, T_7 was found to be the best candidate for elimination and the most sensitive model was obtained by combining T_7 with T_{16}. Table 2 shows the sequence of convergence of parameter identification as the number of parameters decreases when noiseless data are being fitted. In this table, the value of the optimized objective function and the estimated variance occasionally increases due to the increase in modeling error incurred by aggregating zones. Table 2 also shows how the value of the trace of the covariance matrix decreases as the number of parameters is reduced. This reduction of the value of the trace of the covariance matrix indicates a decrease of the value of the individual variances of the parameters. Also, the numerical properties of the sensitivity matrix improved as the number of parameters decreased. This is evident by the fact that the value of the determinant of the sensitivity matrix increases with each reduction on the number of zones reducing the propagation of roundoff error during the inversion of the design matrix.

The value of the determinant of the sensitivity matrix is a measure of the overall sensitivity of a model, however, individual sensitivity coefficients are more useful when visualizing the sensitivity of individual parameters of the model.

Table 2

Comparison of Effects of Reducing the Dimensionality of T on Parameter Reliability Measures Based on the Theoretical Approximation of Covariance Matrix from Inversion of Noiseless Head Data

$\sigma_h = 0.0$					
No. of Zones	**Objective Function**	**Estimated Variance**	**Std. Error for Zone 1**	**Determinant of Matrix A**	**Trace of Cov. matrix A**
36	2.40989E-03	2.409894E-03	4.44499E+06	0.0(*)	1.024843E+17
35	2.91917E-04	1.459583E-04	3.32149E+06	0.0(*)	8.468124E+16
34	1.49796E-04	4.993195E-05	4.61132E+06	0.0(*)	3.153145E+16
33	4.21363E-05	1.053407E-05	1.38838E+06	0.0(*)	5.335440E+12
32	1.09772E-05	2.195430E-06	3.61504E+05	0.0(*)	2.103748E+11
31	2.14981E-04	3.583012E-05	2.71977E+05	1.496376E-317	1.737688E+11
30	2.175095-04	3.107278E-05	1.82451E+05	1.286488E-304	1.367072E+11
29	3.67206E-05	4.595007E-06	5.04948E+04	3.662425E-289	3.302324E+09
28	1.18429E-04	1.315873E-05	5.02427E+02	2.247724E-274	1.511985E+09
27	7.78491E-05	7.784908E-06	3.85768E+02	1.516140E-261	1.702441E+08
26	2.66076E-05	2.418888E-06	3.31017E+01	3.207577E-251	5.079087E+07
25	3.176305-05	2.646921E-06	3.45192E+01	2.426585E-239	3.459053E+07
24	8.95344E-05	6.887260E-06	3.23332E+01	1.009628E-226	3.586827E+07
23	4.08886E-05	2.920615E-06	3.09371E+01	1.884075E-214	6.779037E+06
22	1.31025E-06	8.735029E-08	5.32633E+00	9.908052E-204	1.707379E+05

Figure 13 illustrates the changes in value of the normalized sensitivity coefficient for zone 1. This zone was chosen in this discussion because it is easily traceable during the zonation process. Other zones affected by the zonation did not necessarily maintain their original number as they were combined with neighboring zones. As shown in this figure, the value of the normalized sensitivity coefficient sharply increased an order of magnitude each time a zone was aggregated to zone 1. This occurred twice at $p = 28$ and $p = 26$. Figure 14 shows, in a three-dimensional coordinate system, the increase of the influence of the sensitivity coefficient for zone 1 every time a neighboring zone was aggregated to zone 1.

Parameter zonation was applied in this example until the number of parameters was reduced to 22 transmissivity zones. Table 3 shows the final identified parameters, corresponding standard errors and 95 percent confidence limits. Although further parameter reduction could be applied, this final set of parameters achieved convergence near their exact values and produced small standard errors of the estimates. Notice that there are some parameters with relatively large variances, namely the transmissivity for zone seven. Further elimination of this or any other parameter from the regression would lead to no substantial benefits in terms of increasing the reliability of the identifiable parameters. For this reason, the cut off point to determine the best set of parameters was the set of parameters of reduced dimension which significantly reduced the variances of the estimates and met the convergence criteria used in the optimization. The final parameter distribution for the 22-parameter aquifer is shown in Figure 15.

Close examination of the correlation coefficients for the converged parameters of the model with 22 transmissivity zones, indicated no substantial high correlation for zone 7 with other parameters. This zone has the highest standard error as indicated in Table 3. Under the proposed algorithm, elimination of this parameter would be possible only by combining this zone with either zone 5 or 13, however there is no high correlation

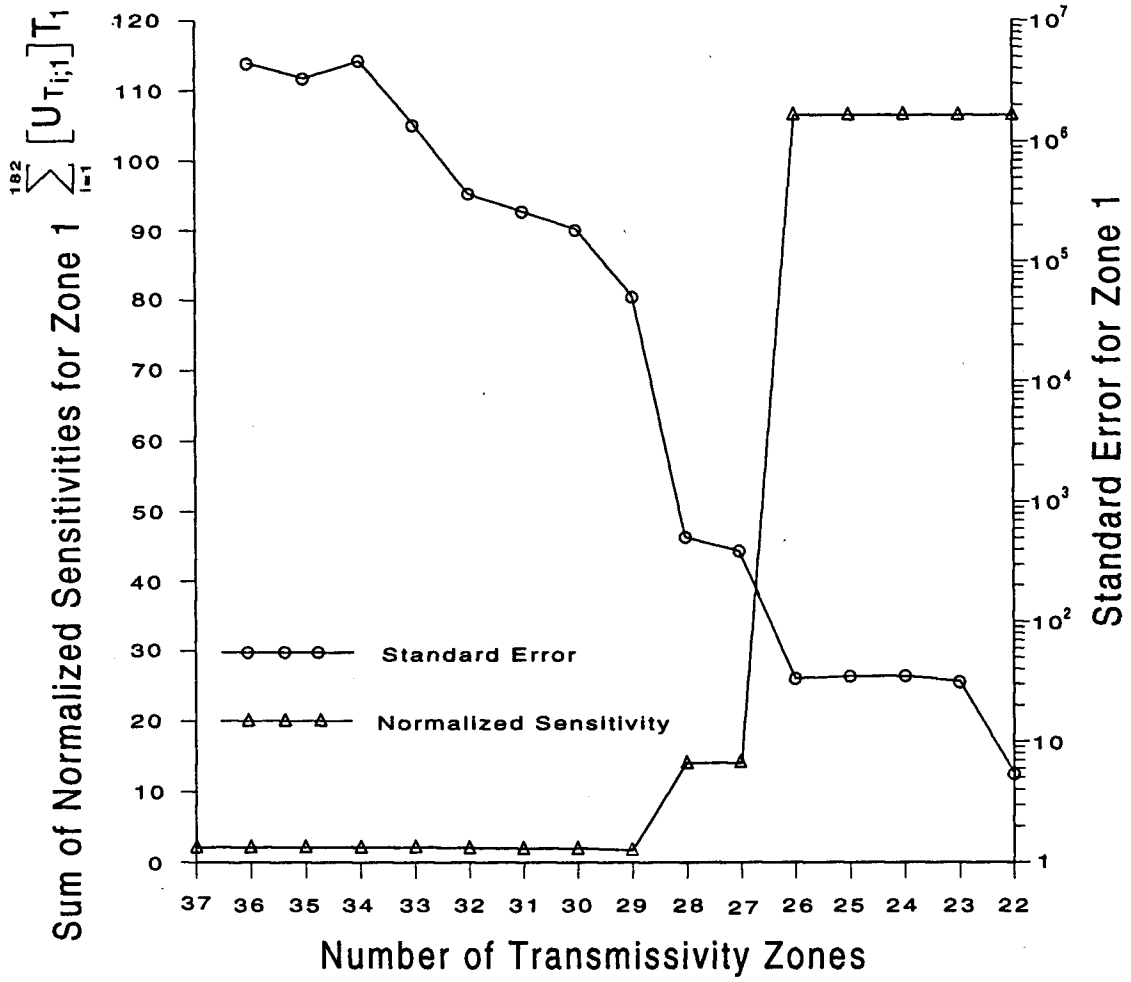

Figure 13. Variation of Sum of Normalized Sensitivities and Standard Errors for Zone 1 with Decreasing Parameter Dimension from Inversion of Noiseless Head Data

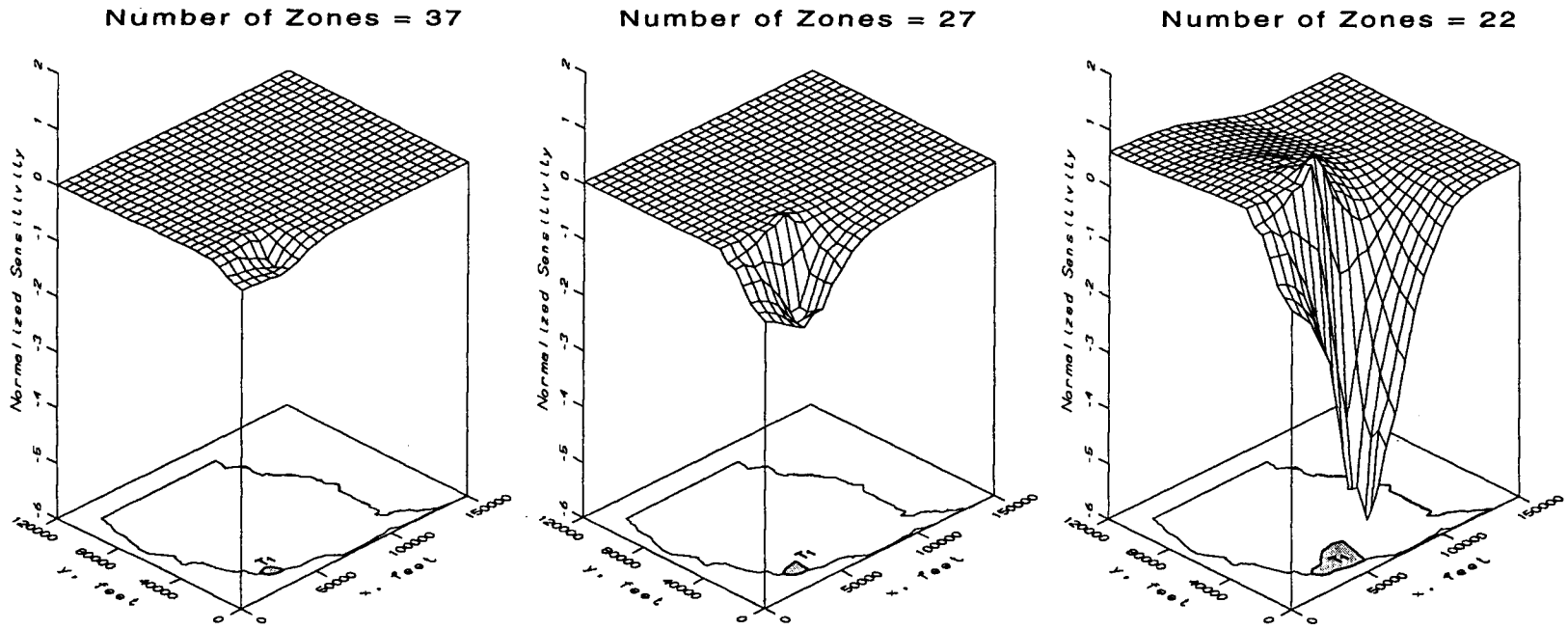

Figure 14. Spatial Influence of Normalized Sensitivity Coefficients for Zone 1 for Parameter Dimension of 37, 28 and 26 Zones

Table 3
Estimated Transmissivities and 95 Percent Confidence Intervals for Error-Free Inversion Data for Model with 22 Transmissivity Zones

Zone	Lower Limit	Estimated T	Upper Limit	Std. Error
1	108861	108872	108883	5.326
2	108857	108870	108884	6.261
3	33489	33499	33509	4.785
4	33495	33500	33505	2.471
5	669955	670016	670077	28.620
6	108865	108870	108876	2.533
7	669471	670056	670641	274.574
8	108790	108936	109082	68.358
9	108784	108851	108918	31.406
10	108836	108952	109069	54.599
11	108835	108862	108888	12.410
12	108583	108752	108922	79.632
13	669818	670013	670208	91.478
14	108835	108875	108916	18.920
15	108819	108865	108911	21.498
16	108797	109013	109230	101.592
17	108204	108598	108992	184.724
18	108728	108863	108999	63.761
19	108828	108873	108919	21.442
20	108857	108877	108897	9.275
21	108581	108885	109189	142.726
22	108821	108875	108928	24.969

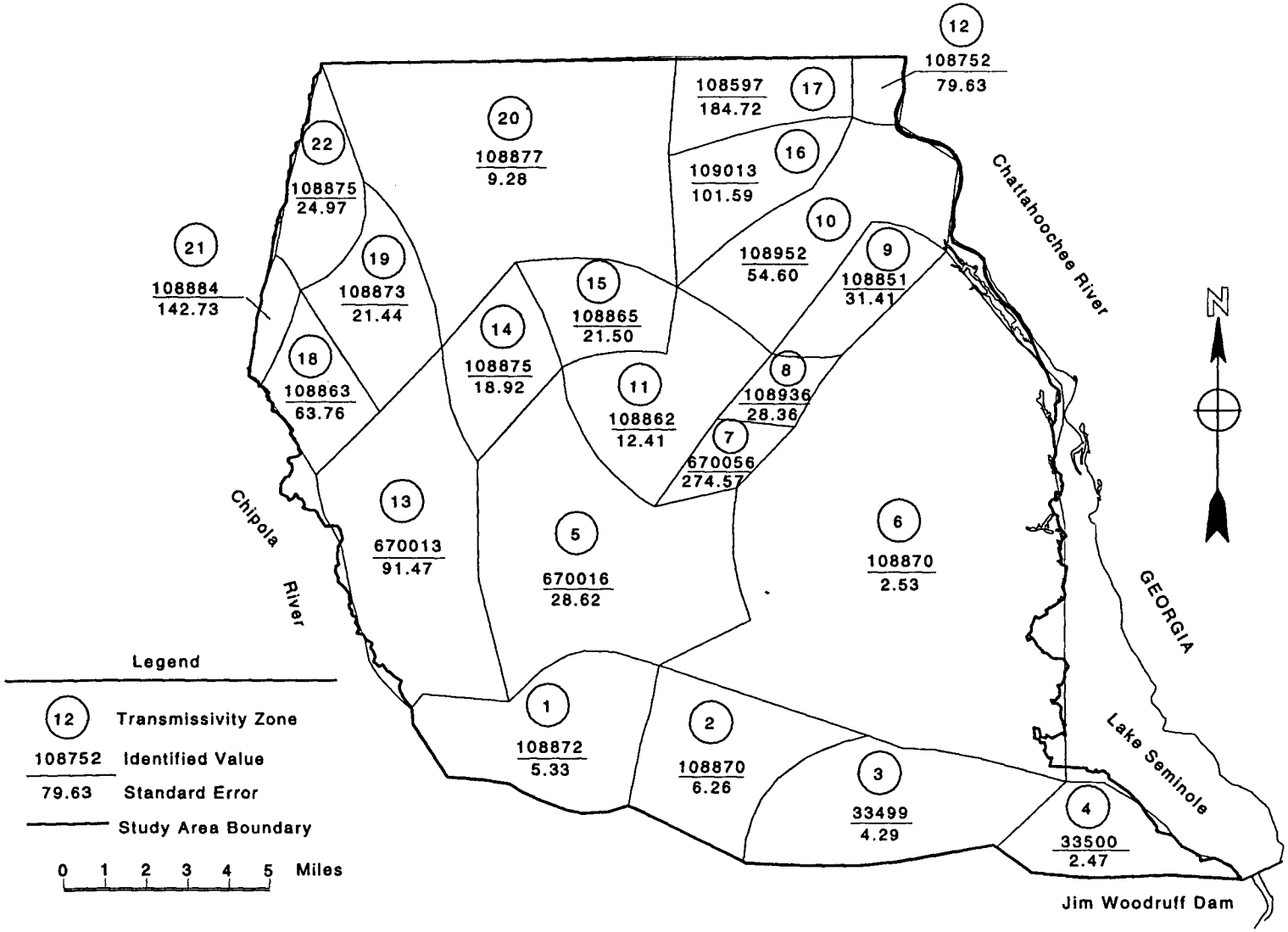

Figure 15. Identified Zonal Transmissivities from Inversion of Noiseless Head Data

between the transmissivity in zone 7 with either of these zones. Combining this parameter with any other zone would lead to a drastic increase in the value of the objective function and is greater than the allowable value of ten times the value of the objective function for the previous iteration. This value was determined experimentally and performs reasonably well when defining zonation patterns, without leading to divergence of the solution. The main reason for this parameter is to maintain the value of the objective function close to the value of the objective function from the previous iteration. Therefore, eliminating zone 7 would not significantly reduce the variance of the estimates making unnecessary further parameter eliminations from the final model with 22 parameters since convergence to the solution has been achieved.

A not surprising fact is that the final zone 6 had the second smallest standard error in the final model. This zone was initially formed by grouping several elements into a large zone due to the lack of head data near or in the zone. This suggests that the elimination of redundant parameters from the solution, even before the model is optimized, can be beneficial in terms of more reliable identified parameters.

Inversion of Noisy Head Data

In this section, the effects of data error are considered in estimation accuracy and parameter identifiability assuming that the correct constitutive model is employed in the inversion, but input data are subject to random error. In this example, correctness in the model implies that there is no error in model representation of boundary conditions, inflows, outflows, and spatial distribution of the parameters in the form of zones of constant transmissivity value. Data error may be regarded as representing the effects of measurement error by a $N(0,\sigma_h^2)$ term which is added to the heads at each observation point. Two different data sets of corrupted heads with error standard deviations of 0.2236

and 1.0000 feet were considered. These are rather large errors chosen to represent cases of severe measurement uncertainty.

For both cases, head data corrupted with noise with $\sigma_h = 0.2236$ and $\sigma_h = 1.0$, attempts to solve the inverse problem with all 37 transmissivity zones as unknown parameters resulted in unstable solutions. A more relaxed convergence criterion led to solutions with very large standard errors on the parameters. Furthermore, these solutions depended greatly on the starting value of the parameters. In other words, the problem no longer has a unique solution. However, direct information on some of the parameters is available from the experiment itself which can be used to reduce the dimensionality of the parameter set. This information, specifically about the magnitude of the sensitivity coefficients at the sampling points, is used during the optimization procedure to eliminate redundant parameters or parameters that cannot be identified accurately. The application of the parameter elimination techniques proposed in chapter four to these two examples led to a solution vector consisting of 19 parameters for the case of head data corrupted with noise with variance (σ_h^2) of 0.05. For the case of head data corrupted with noise with standard deviation of 1 foot the final set of parameters consisted of 21 transmissivity zones. Figures 16 and 17 respectively show the final transmissivity zone distributions for these two examples with noisy data. These two figures along with Figure 15 demonstrate the fact that the number of parameters that can be meaningfully identified decreases as the level of uncertainty increases. In these examples with corrupted head data, additional parameter eliminations from the solution would not further reduce uncertainty in the system because elimination of additional parameters would increase the error from coarsening the transmissivity zones. The only possible remedies to this problem would be to include additional information in the objective function, either in the form of prior information about the parameters, or in the form of additional head observations in the

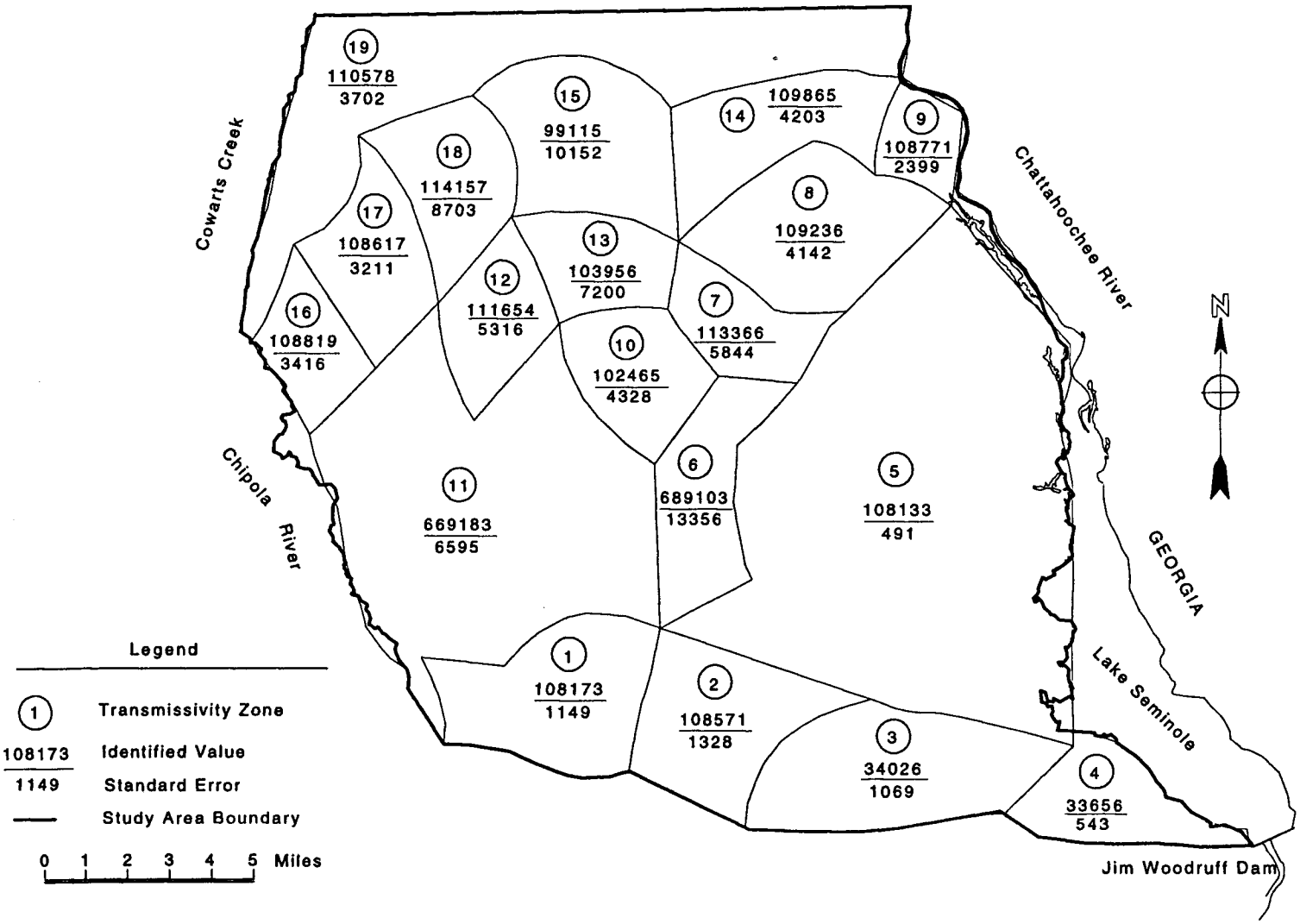

Figure 16. Identified Zonal Transmissivities from Inversion of Head Data Corrupted with Noise (N,σ^2 = 0.05)

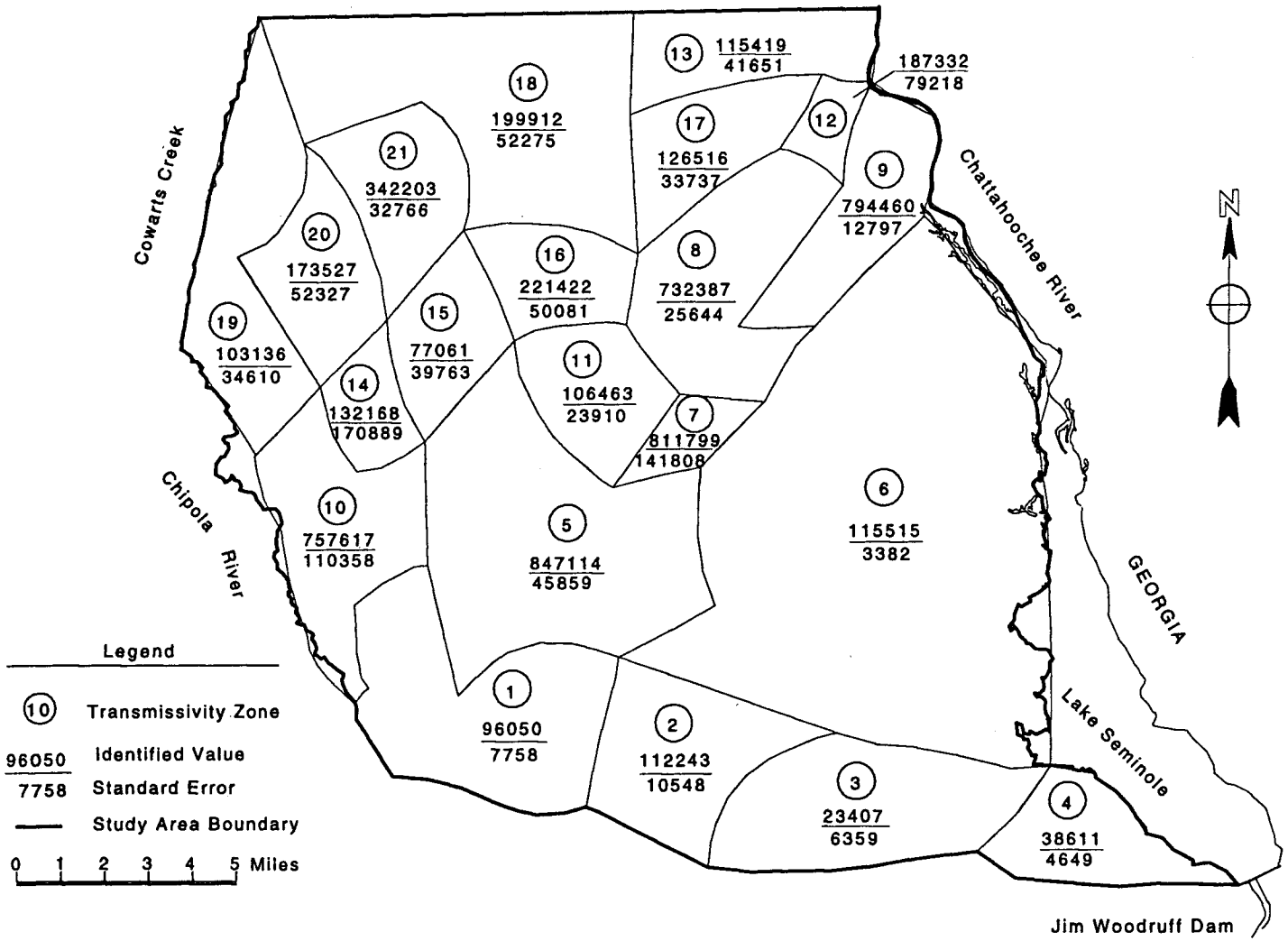

Figure 17. Identified Zonal Transmissivities from Inversion of Head Data Corrupted with Noise (N, σ^2 = 1.00)

regression. The effects and limitations of these remedies have been presented in previous studies [Carrera and Neuman, 1986; Chu et al., 1987].

Analyses of the statistics for the corrupted data regressions are shown in Tables 4 and 5. As in Table 1 for the case of noiseless data, the elimination of ill-defined parameters applied during the minimization of the objective function have a positive effect on the trace of the covariance matrix, the objective function, the parameter variance and the standard error of the parameters. Figures 18 through 21 illustrate the effects of the transmissivity zonation summarized in Tables 2, 4 and 5. In Figure 18 the value of the objective function and the estimates variance is plotted versus the number of transmissivity zones in the regression model for all three sets of data. For the noiseless data case, the value of the objective function was reduced from 2.5953E-02 for the 37 zone model to 1.3103E-06. Intermediate oscillations in the value of the objective function are due to the fact that different models have a different degree of convexity in the objective function. However, by allowing more iterations in the minimization process or starting at a different initial point, these intermediate models could yield smaller values of the objective function than models with more parameters. In the case of noisy data with $\sigma_h^2 = 0.05$, the minimum value of the objective function occurs when the number of parameters in the model, p, equals 35. Additional elimination of parameters increased the value of the objective function from a minimum of .009225 to .0747 suggesting that the error component in the objective due to coarsening of the transmissivity zones increases as the number of zones decreases even though the error component due to statistical uncertainty decreases as suggested by the decreasing value of the trace of the covariance matrix (Figure 19). At this noise level, the minimum value of the parameter variance occurred at an intermediate number of zones (p = 29). When the noise in the head data was increased to $\sigma_h^2 = 1.0$, parameter elimination from the regression did not have a

significant effect on the value of the objective function suggesting that the noise in the head data overpowers the error from the coarsening of the transmissivity zones. Elimination of parameters from the regression did not significantly decrease the parameter variance for p less or equal to 26 as shown in Figure 18 .

The effect of reducing the numbers of parameters from the regression on the trace of the covariance matrix is shown in Figure 19 for noiseless and noise-corrupted head data. In all three cases the value of the trace is reduced with each parameter elimination. The greater reduction in the value of the trace of the covariance matrix occurs during the first stages of the zonation process. This is due to the fact that the zonation algorithm was designed to sequentially eradicate from the regression the parameter with largest variance.

Figure 20 shows the effect of parameter elimination on the standard error of zone 1. This zone was chosen for illustrative purposes because it was easily traceable as zonation is applied to the model and zones combine with each other. Because the standard errors of the regression parameters are related to the diagonal elements of the covariance matrix, the standard errors follow a similar pattern as the trace of the covariance matrix with largest reductions in their value during the initial stages of the zonation.

The numerical properties of the matrix A are improved with each parameter elimination, as indicated by the decrease of the value of the determinant of the matrix A as the number of parameters decreases. This is shown graphically in Figure 21 where, for all three cases of noise level in the head data, increased values of the condition number were obtained with smaller sets of parameters. For singular matrices and near-singular matrices at the initial stages of the zonation process, the determinant was not defined at the working precision of the computer.

Table 4.

Comparison of Effects of Reducing the Dimensionality of T on Parameter Reliability Measures. Based on the Theoretical Approximation of the Covariance Matrix [From Inversion of Head Data Corrupted with Noise $N(0,\sigma_h^2 = 0.05)$].

$\sigma_h^2 = 0.05$					
No. of Zones	**Objective Function**	**Estimated Variance**	**Std. Error for Zone 1**	**Determinant of Matrix A**	**Trace of Cov. matrix A**
36	2.25417E-02	2.254172E-02	4.45078E+06	0.0(*)	2.148859E+17
35	9.22569E-03	4.612843E-03	3.48622E+06	0.0(*)	1.520990E+15
34	9.22761E-03	3.075870E-03	4.05665E+05	0.0(*)	1.777334E+12
33	7.05776E-02	1.764440E-02	1.93910E+05	0.0(*)	1.501010E+12
32	1.07591E-02	2.151837E-03	1.26642E+04	0.0(*)	5.017425E+11
31	1.08560E-02	1.809338E-03	9.59950E+03	2.712622E-311	4.117172E+11
30	1.07981E-02	1.542588E-03	8.58098E+03	2.653953E-297	1.988129E+11
29	1.05559E-02	1.319487E-03	7.95708E+03	1.139503E-285	1.198381E+11
28	3.58154E-02	3.979490E-03	2.63716E+03	3.893008E-275	8.665953E+10
27	2.76650E-02	2.765054E-03	2.19182E+03	3.668186E-262	5.351871E+10
26	2.80535E-02	2.550320E-03	2.00241E+03	5.757855E-250	2.393187E+10
25	3.16487E-02	2.637392E-03	1.37124E+03	2.820606E-238	2.225319E+10
24	3.29047E-02	2.531127E-03	1.28819E+03	1.051042E-226	1.686283E+10
23	6.84349E-02	4.888206E-03	1.43426E+03	2.866702E-214	1.171052E+10
22	6.84713E-02	4.564754E-03	1.35694E+03	3.421169E-204	9.774351E+09
21	6.86208E-02	4.288801E-03	1.31260E+03	4.149202E-192	5.120244E+09
20	7.15912E-02	4.211245E-03	1.20041E+03	4.167890E-180	1.025468E+09
19	7.47068E-02	4.150381E-03	1.14913E+03	2.597164E-170	6.145217E+08

Table 5.

Comparison of Effects of Reducing the Dimensionality of T on Parameter Reliability Measures. Based on the Theoretical Approximation of the Covariance Matrix [From Inversion of Head Data Corrupted with Noise $N(0,\sigma_h^2 = 1.00)$].

$\sigma_h^2 = 1.0$					
No. of Zones	**Objective Function**	**Estimated Variance**	**Std. Error for Zone 1**	**Determinant of Matrix A**	**Trace of Cov. matrix A**
36	3.02275E+00	3.022747E+00	4.48756E+06	0.0(*)	1.361437E+20
35	3.05440E+00	1.527200E+00	2.59733E+06	0.0(*)	2.831415E+19
34	3.12384E+00	1.041279E+00	2.11890E+06	0.0(*)	4.581876E+19
33	3.00540E+00	7.513511E-01	1.84291E+06	0.0(*)	1.300400E+19
32	3.09927E+00	6.198534E-01	1.64930E+06	0.0(*)	4.720917E+15
31	3.02381E+00	5.039679E-01	1.51948E+06	2.298788E-315	9.799466E+14
30	3.01959E+00	4.313706E-01	1.36696E+06	3.255706E-302	4.413684E+14
29	3.01088E+00	3.763596E-01	6.97435E+04	5.560344E-288	2.667941E+14
28	3.24227E+00	3.602523E-01	9.41720E+03	1.761177E-277	3.159196E+14
27	3.27491E+00	3.274915E-01	9.08941E+03	5.135172E-265	6.928641E+13
26	3.24794E+00	3.024472E-01	8.72735E+03	4.139022E-255	5.353995E+13
25	3.32884E+00	2.774029E-01	8.36530E+03	3.918012E-241	3.773927E+13
24	3.39076E+00	2.608278E-01	8.15207E+03	1.371202E-226	1.120510E+12
23	3.75325E+00	2.680891E-01	8.29079E+03	1.988836E-216	9.160065E+11
22	3.62034E+00	2.413561E-01	7.95622E+03	1.118063E-205	3.230512E+11
21	3.65162E+00	2.282265E-01	7.75718E+03	3.500983E-195	3.121161E+11

(*) - Zero at single precision arithmetic

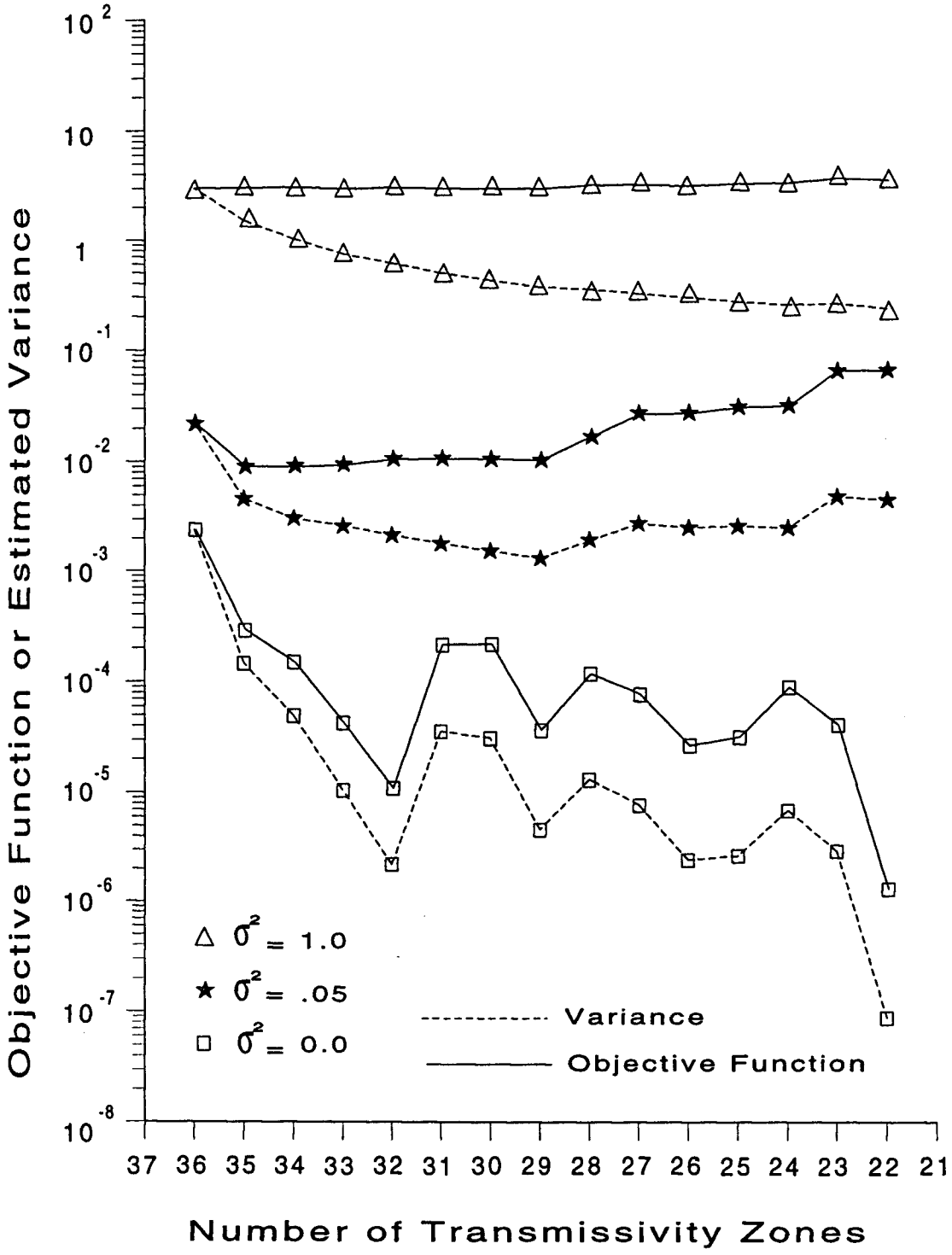

Figure 18. Variation of Optimized Objective Function and Estimated Head Variance with Decreasing Parameter Dimension

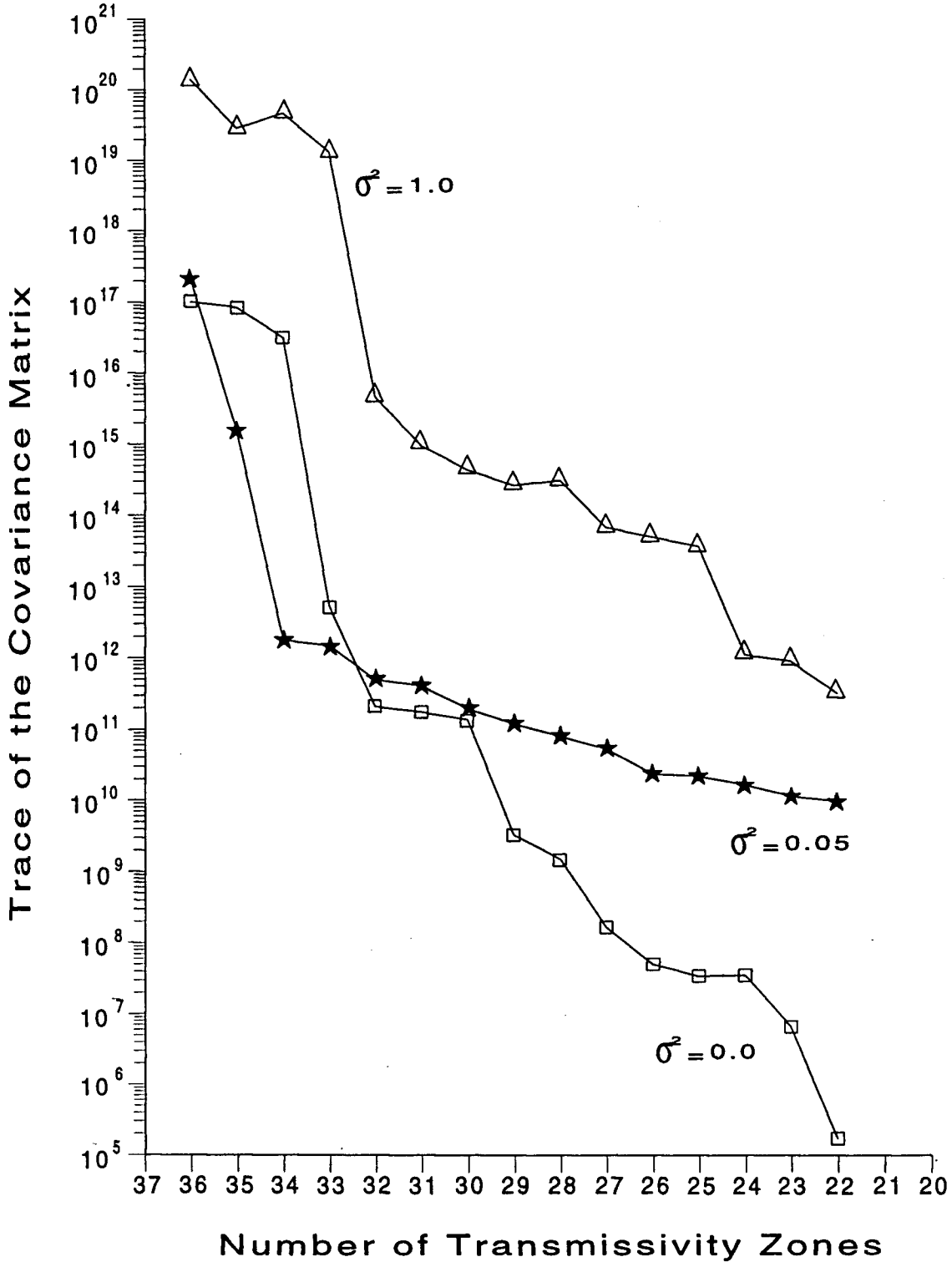

Figure 19. Variation of the Trace of the Covariance Matrix with Decreasing Parameter Dimension

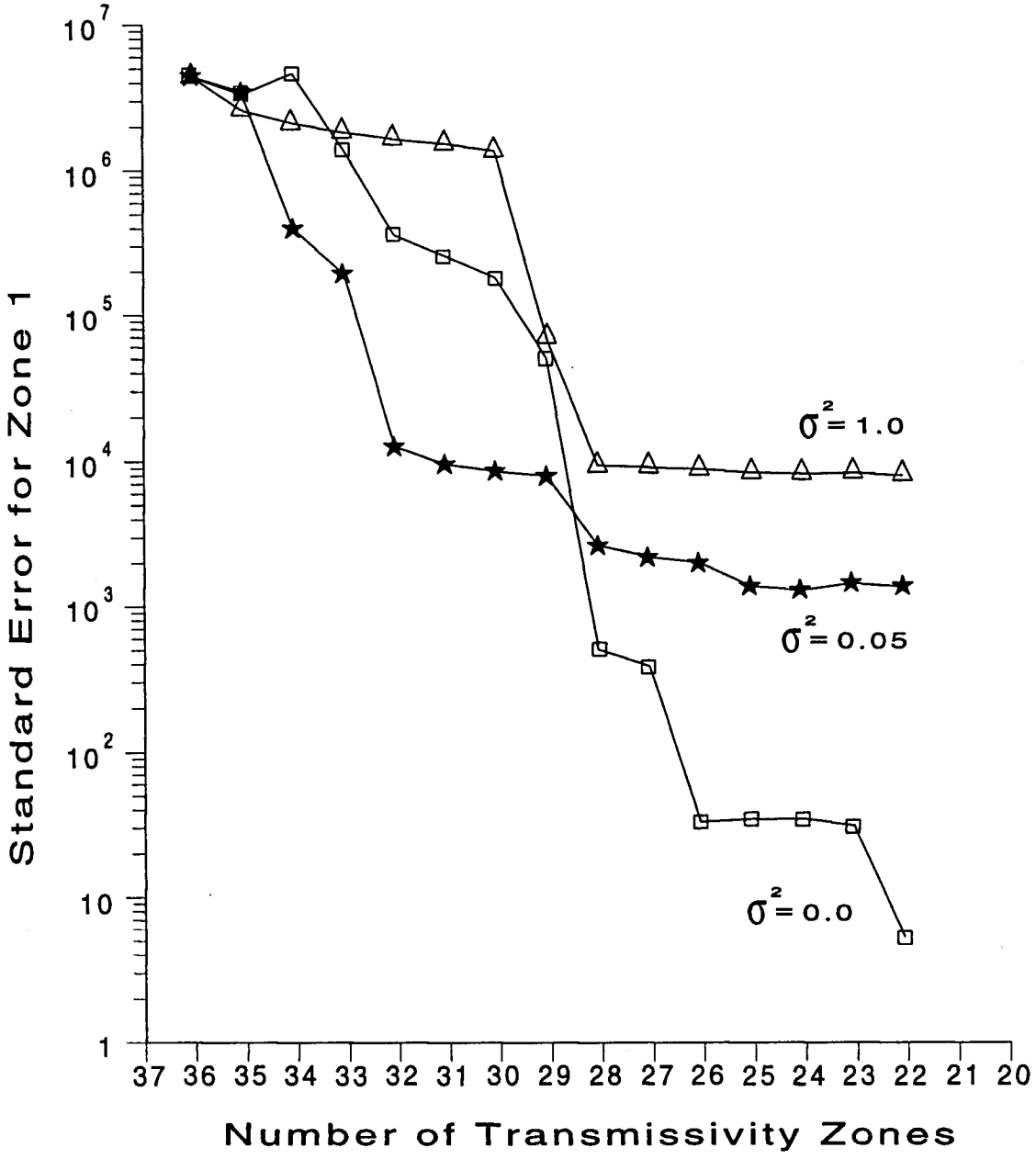

Figure 20. Variation of Standard Error of Transmissivity in Zone 1 with Decreasing Parameter Dimension

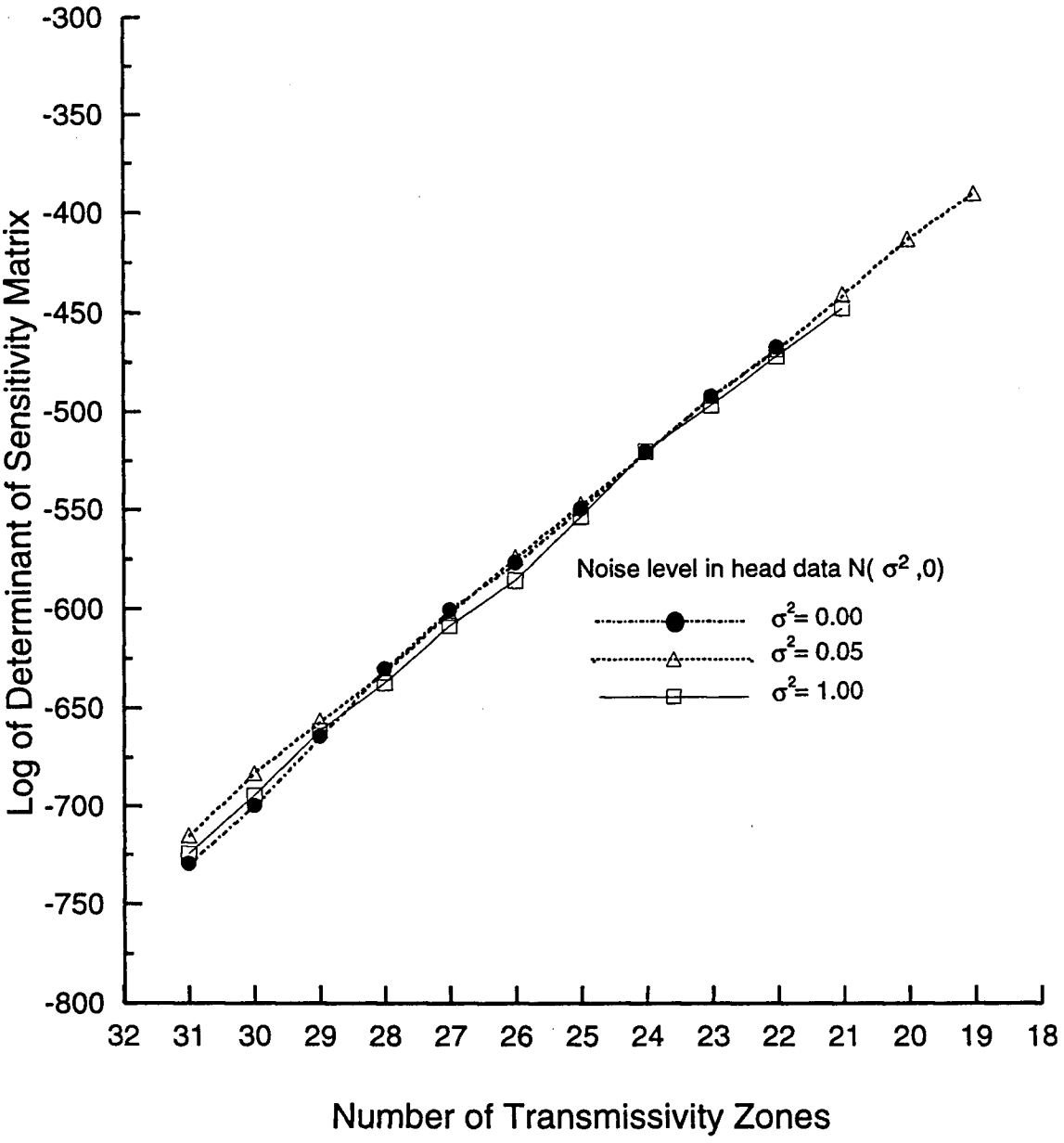

Figure 21. Variation of the Log of the Determinant of the Sensitivity Matrix with Decreasing Parameter Dimension

Inversion of Field Head Data

The last application of the proposed methodologies, is the inversion of a set of head data with real field noise characteristics. In this exercise the same aquifer configuration, boundary conditions, inflows, outflows, and number and location of observation wells were employed as in the previous examples (Figure 10). The initial transmissivity zone distribution and values used as starting conditions for the optimization and zonation processes were identical to the previous examples with synthetic head data. The main reason for using the same initial values was to make a direct comparison of the convergence performance of the algorithms at different noise levels. The head data utilized in this example is from the data set obtained during the wet season, May-July, 1989 (Figure 7). Although 72 head observations were made during this sampling period in the study area, only 37 head observations were considered accurate and included in the regression (Figure 10). Since observation error can have a severe impact on the identified parameters, it was necessary to eliminate from the regression the observations with largest uncertainties. A confidence weighting factor could not be applied to the erroneous observations because there was no record associated with the reliability of each observation. Therefore, head outliers were simply identified from historical head potentiometric maps. Only those values that closely followed historical head patterns were included in the regression. The results from the application of the zonation algorithm to the inversion of this data set is summarized in Table 6. This table shows the converged value of the objective function, variance of the predicted heads, determinant and trace of the covariance matrix for models with a decreasing number of transmissivity zones. Sequential elimination of ill-defined parameters from the solution led to a model with 24 transmissivity zones. The reduction in the value of the optimized objective function between parameter eliminations is relatively small. This suggests that careful selection of ill-conditioned parameters together with proper

combination of zones can lead to an equally good or better model in term of their variances. As in the examples with synthetic head data, the algorithm consistently enhances the numerical properties of the matrix A during inversion as shown by the increasing value of the determinant of the sensitivity matrix. The final transmissivity distribution with 24 zones is shown in Figure 22. This figure shows several parameters with relatively large variances such as zones 5, 8, 9 and 24. In all these instances the standard error was larger than the identified value.

Several attempts were made to eliminate these parameters, however, further parameter elimination from the solution invariably led to an increase of the value of the objective function to a non-permissible level preset in the algorithm to avoid numerical instability.

Table 6
Comparison of Effects of Reducing the Dimensionality of T on ParameterReliability Measures. Based on the Theoretical Approximation of the Covariance Matrix (from Inversion of Field Data).

No. of Zones	Objective Function	Estimated Variance	Determinant of Matrix A	Trace of Cov. matrix A
36	1.01999E+02	1.019997E+02	0.0 (*)	3.851630E+20
35	1.01263E+02	5.063174E+01	0.0 (*)	1.189373E+19
34	1.01180E+02	3.372666E+01	0.0 (*)	7.054729E+18
33	1.00995E+02	2.523627E+01	0.0 (*)	2.193936E+18
32	1.00740E+02	2.014796E+01	0.0 (*)	2.835928E+17
31	9.96681E+01	1.661135E+01	6.789401E-299	2.308885E+16
30	9.85334E+01	1.407021E+01	1.547688E-286	1.371601E+16
29	9.74414E+01	1.218018E+01	7.317184E-272	3.072323E+15
28	9.70726E+01	1.078585E+01	2.030338E-257	8.871605E+13
27	9.53867E+01	9.533867E+00	5.141579E-245	5.242957E+13
26	9.51737E+01	8.652152E+00	2.587502E-233	2.700405E+13
25	9.47463E+01	7.871917E+00	1.365692E-223	2.542192E+13
24	9.36557E+01	7.024288E+00	3.092692E-211	9.540449E+12

(*) - Zero at single precision arithmetic

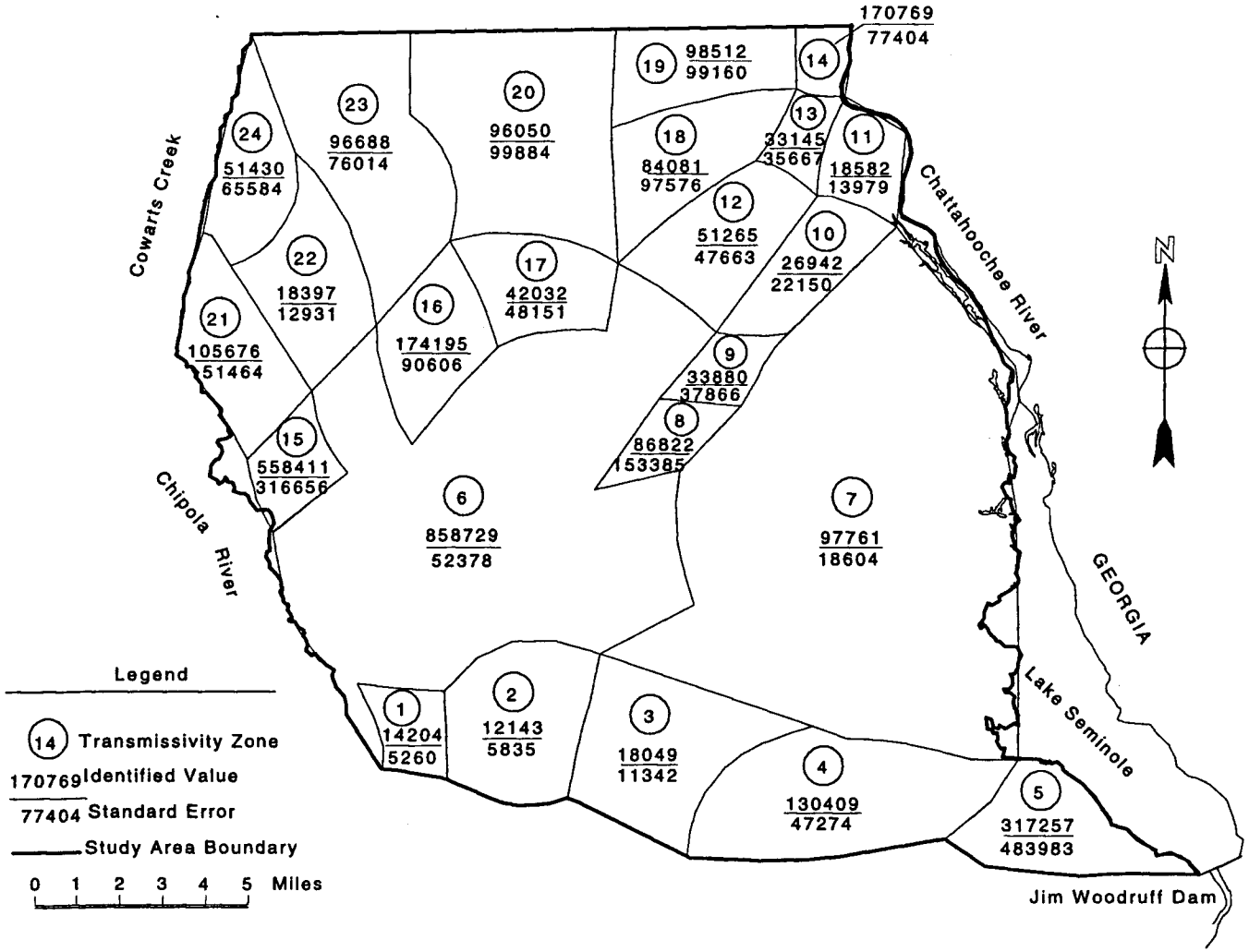

Figure 22. Identified Zonal Transmissivities from Inversion of Field Data

In this case, one possible way to further enhance the quality of the identified parameters may be to add head data of good quality into the solution, or prior information about the parameters. Figure 23 shows a three-dimensional view of the identified transmissivity distribution and the corresponding head distribution. These figures clearly show the zone of high transmissivity around the Blue Spring which coincides with previously calibrated transmissivities for this area [Roaza, 1989]. Such drastic changes in the value of the transmissivity from one region to another are characteristic of severely weathered limestones in which flow through secondary porosity features is the prevalent mechanism to water movement in the aquifer. It is in this area of high transmissivity where the zonation algorithm found most of the ill-defined parameters and where most of the zonation adjustments occurred. This can be attributed to the relative low head gradient and lack of informative head data in the region. Refinement of the finite element mesh in this area and inclusion of additional head data into the regression may result in a better conditioned model.

Figure 24 shows the comparison of the fitted head distribution with the 24 zone model and the observed data. Figure 25 shows the residual distribution over the study area. The absolute value of the maximum, minimum and mean residuals are 4.53 feet, 0.13 feet, 0.26 feet respectively, and the standard deviation 1.59 feet. As expected, the largest head residuals lie within the eastern part of the aquifer where head data are scarce. The other area with large residuals, possibly due to a zone of low hydraulic gradient, is near the Blue Spring area, near the 80-foot contour line.

The identified transmissivity distribution, even though it produces a good match between observed and simulated heads, contains parameters with large uncertainties. However, further enhancement of the solution can be achieved with information that can be inferred from this model such as locations for additional informative wells and further refinement of the zones in areas of the model with large uncertainties.

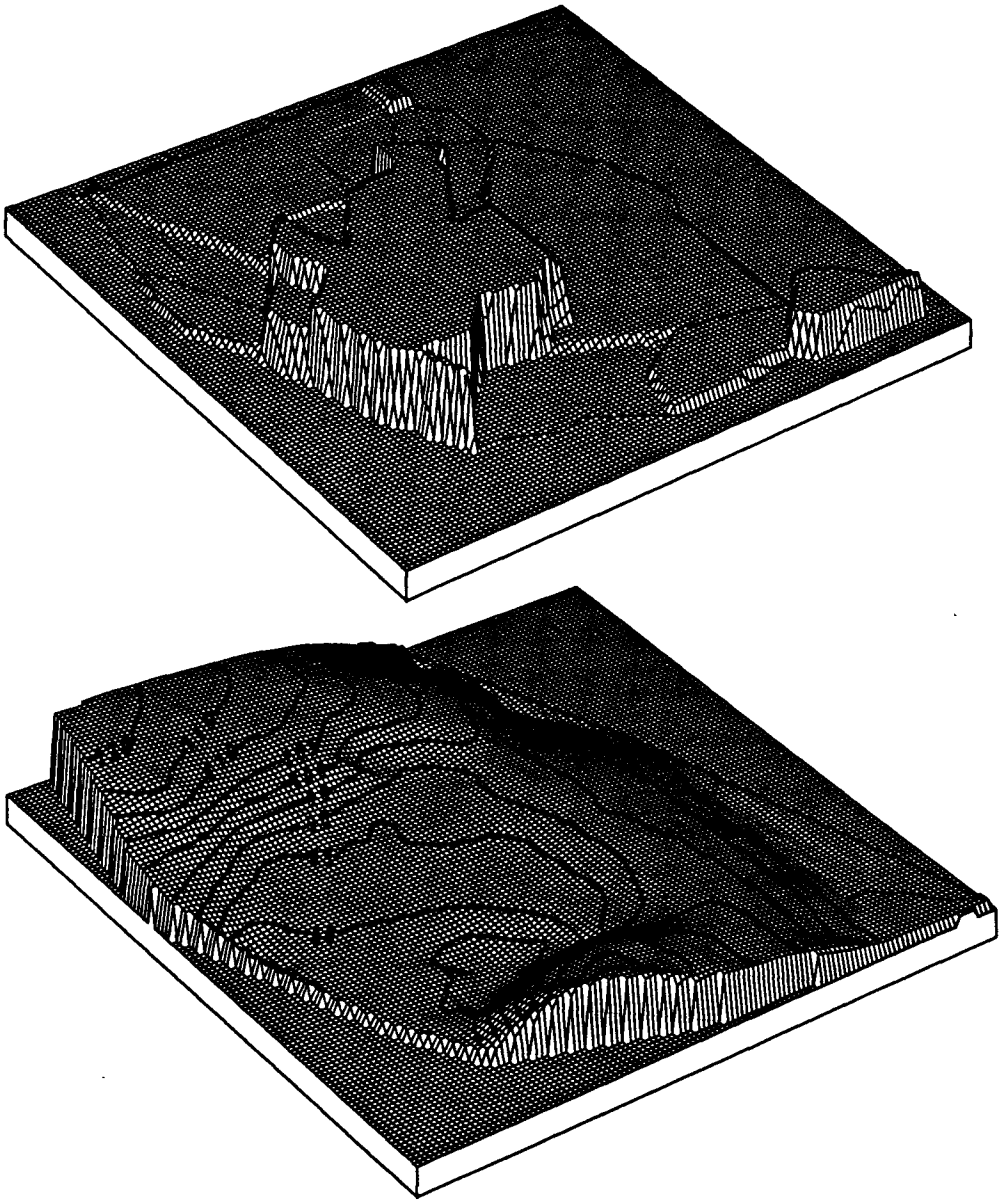

Figure 23. Three-Dimensional Map of Identified Transmissivities and Head Potential Over the Study Area

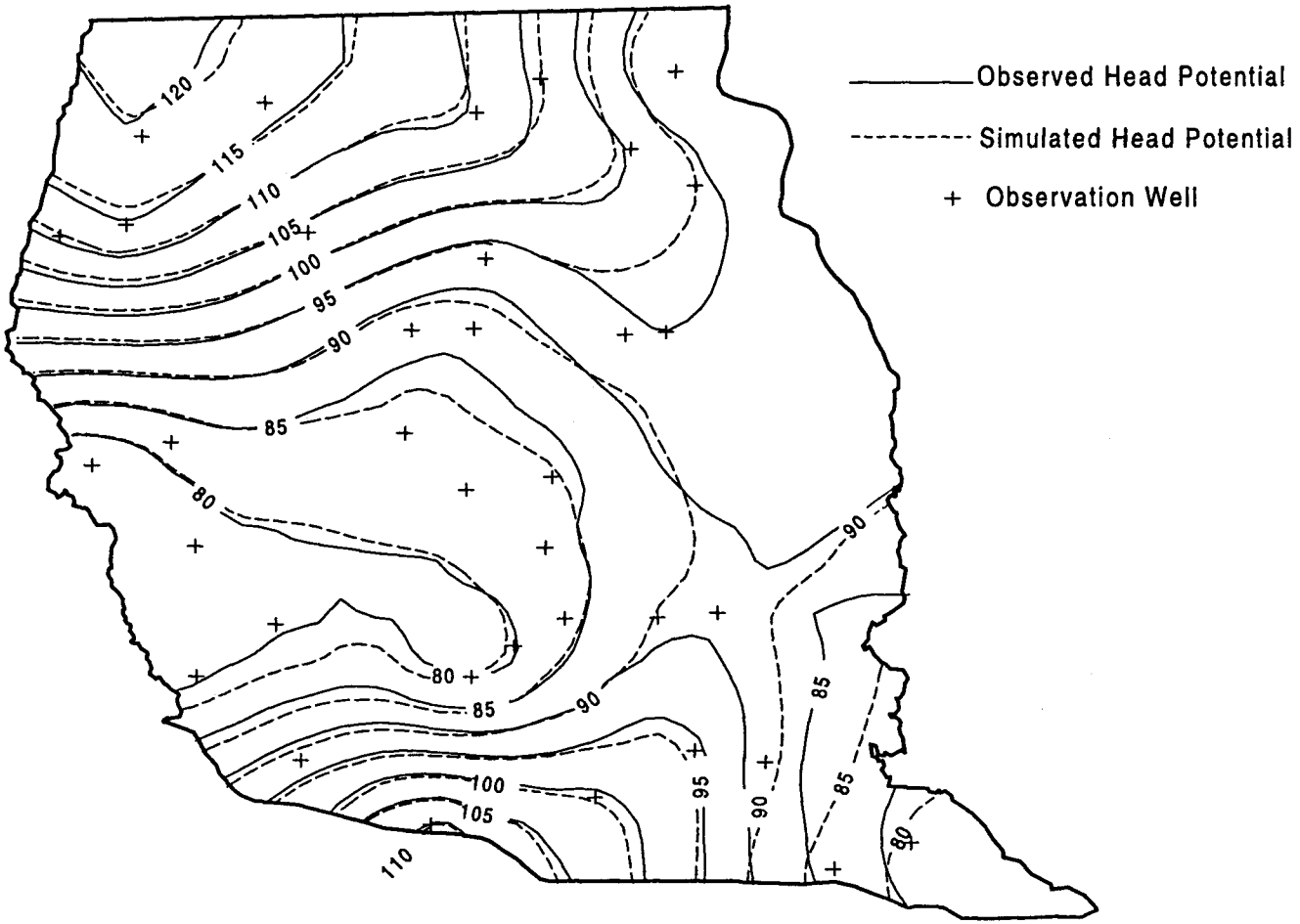

Figure 24. Head Residual Contour Map from Inversion of Filed Data

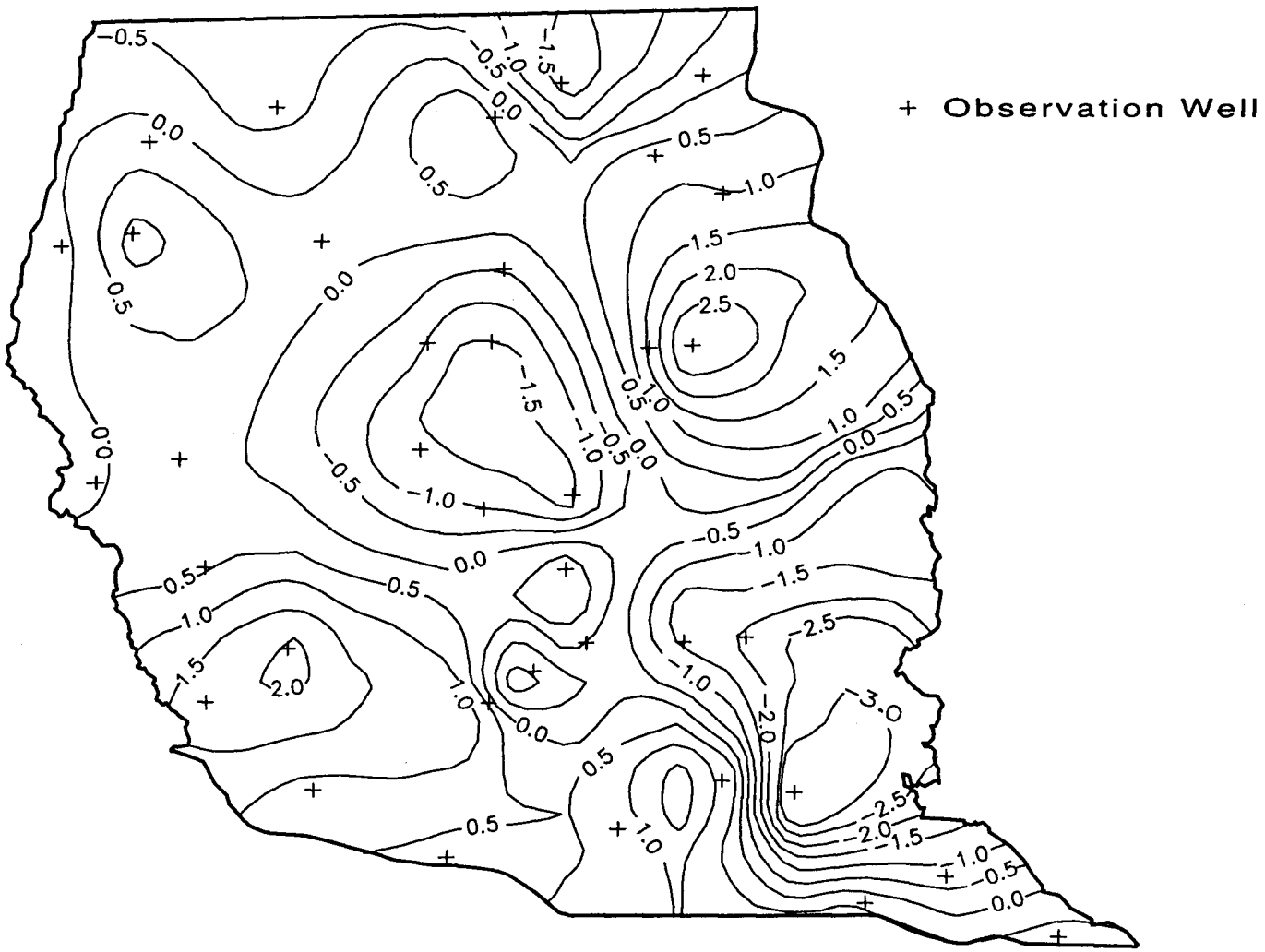

Figure 25. Head Residual Contour Map from Inversion of Field Data

CHAPTER 6

SUMMARY AND CONCLUSIONS

The ill-posedness of the groundwater inverse problem remains a difficulty for modelers in the calibration of groundwater numerical models. However in the last few years, considerable progress has been made in understanding its causes, effects, and the circumstances under which a solution may be attainable for practical problems.

In this study, an indirect method of solution was chosen over the direct approach because of the flexibility of indirect methods in dealing with inadequate and scarce data. The resulting parabolic-type equation is solved with optimization methods, formulated in terms of the least squares minimization of residuals.

Several techniques to deal with the ill-posedness of the problem were investigated. Identifiability can be achieved in practical applications by relaxing the identifiability criteria [Yeh, 1986]. When more parameters are being identified than the amount of information provided by the head data allows, instability and non-uniqueness often results. Therefore, controlling the parameter dimension is an important step toward a more stable and unique solution. Techniques such as application of constraints in the estimates, log transformations of the parameters, inclusion of prior information, and reparameterization of the transmissivity distribution have showed their usefulness in controlling the ill-effects of instability and nonuniqueness during the solution.

For this study, a modified Marquardt method of minimization was used to seek the solution. Marquardt's method of minimization has demonstrated its efficiency and robustness in dealing with ill-conditioned nonlinear problems. This method employs two scalar functions: μ, which enhances the numerical properties of the design matrix to allow inversion without difficulties, and ρ, which scales the length of the correction step to induce convergence. Prior information about the parameters was included as part of the

optimization method in the form of linear constraints in the parameters by the penalty function method. This method of imposing constraint information into the objective function was easily incorporated into Marquardt's algorithm making the modified minimization algorithm more capable of dealing with ill-posed problems.

Nonuniqueness of the problem is a common symptom of the ill-posedness characteristics of the inverse problem. It arises in many practical problems when parameters are being identified in zero or near zero hydraulic gradient areas or in areas of zero or near zero sensitivity such as constant head boundaries. A method to circumvent this problem is to reduce the number of parameters from the solution. One convenient way of achieving this is by determining the value of the parameter from observations so that it can be eliminated from the solution. This, however, is not a feasible alternative for most practical applications since the real form of the transmissivity distribution is unknown. Another alternative is to eliminate from the solution a number of ill-determined parameters until convergence to a reliable set of parameters is achieved. There are two methods of parameterization found in the literature: the interpolation and the zonation methods. In this study we have chosen the zonation method. This method of parameterization has been demonstrated to be very simple to apply and, in many cases, superior to the performance of interpolation methods when inadequate head data is available [Keidser and Rosebjerj, 1991].

The approximation of the head distribution during the optimization process is computed with the finite element method. This method has several advantages over finite differences in the sense that the flow and parameter boundaries can be conveniently fitted using an adequate interpolation basis function for the elements. The computation of sensitivity coefficients is also carried out using the finite element technique and the sensitivity equation method [McElwee, 1985]. Large computational savings result when

using finite elements to solve for the forward solution and the sensitivity coefficients since the same stiffness matrix is used in both solutions.

Linear statistical measures of parameter reliability are used to evaluate the relative worth of the estimates. In this method, zones corresponding to ill-determined parameters are eliminated from the solution by grouping them together with zones corresponding to well-determined parameters. The ill-defined parameters are detected using estimated variances from the theoretical approximation of the covariance matrix. The determinant of the sensitivity matrix is used as a measure of model sensitivity to find the model with largest sensitivity among models of equal number of parameters. These techniques for controlling the dimension of the parameter space were incorporated into the Marquardt method of minimization resulting in an efficient algorithm capable of finding not only the optimum value of the zonal transmissivities but also their structure for a problem with inadequate field data. This reduction of the parameter set dimensions can be applied at any stage of the solution. The reason for this is that ill-conditioning can occur at any stage of the minimization resulting in divergence and instability of the solution. The resulting zonation pattern obtained with this zonation approach yielded a model of reduced dimensions with larger overall sensitivity thus leading to a more stable solution and more reliable estimates of the parameters. This was indicated by increasing values of the determinant of the sensitivity matrix with reduced dimension of the parameter set. Measures of parameter reliability used in this study included the estimated error variance of the heads, standard errors of the estimates and the trace of the covariance matrix

The effectiveness of the proposed algorithms was demonstrated in two numerical experiments. These experiments were carried out for a portion of the Floridan Aquifer in northwest Florida where limited head data were available. Long term stresses in the aquifer were assumed to be in equilibrium with the inflows from recharge. Inflows, outflows, and boundary conditions were evaluated from field data using the most reliable

information. The aquifer was subdivided into 37 transmissivity zones. In the first numerical experiment, a hypothetical head distribution was obtained using a hypothetical transmissivity distribution. This head distribution was then corrupted with Gaussian noise with variance equal to 0.05 ft and 1.00 ft. Then the parameters were identified for all three cases, including the exact head distribution. In the first experiment with noiseless data, the algorithm performed as expected converging near the exact solution. This particular problem was severely ill-conditioned due to the lack of informative head data to identify all 37 parameters, even though exact data was being fitted. After zonation was applied and after 15 ill-determined parameters had been sequentially removed from the solution, the algorithm converged near the exact solution. Most of the parameter deletions occurred, as expected, in areas where non-uniqueness arises due to near-zero head gradients. This experiment shows that under noiseless head data conditions, the zonation procedure can effectively reduce ill-conditioning of the problem to a level where the satisfactory solution can be found.

Under noisy conditions the zonation algorithm was also capable of reducing the dimensionality of the parameter space until convergence to a stable solution was achieved. The effect of reducing the dimension of the parameter set was beneficial in terms of reduced variances of the estimates and other reliability indicators, however, in the case of head data corrupted with high level of noise, the zonation process was applied until further parameter reductions would introduce a large error component due to poor representation of the parameter distribution. This suggests that any further reduction of uncertainty in the estimates would have to come from inclusion of additional data into the model. This was also the case for the inversion of field data. The head data in this case was inadequate for identification purposes in terms of quantity and quality. Despite this, the zonation algorithm was able to reduce the uncertainty of the estimates and converge to a reduced set of parameters. The final fit between the observed and simulated water

levels in the aquifer was characterized by errors ranging from a maximum of 4.53 feet to a minimum of 0.13 feet. The average estimated error in the heads was 0.26 feet. Despite a good fit in the computed heads, large uncertainties about several parameters still remain.

An appropriate topic of subsequent research would be the optimal incorporation of head data into the solution so that direct information on the least sensitive parameters is obtained, enabling either their elimination from the solution, or adequate determination during the inverse process with resulting smaller variances.

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APPENDIX I

MODIFIED MARQUARDT METHOD OF MINIMIZATION

The Marquardt algorithm applied to our groundwater identification problem can be summarized as follows:

1) Consider h a nonlinear function of x, y and T:

$$h(x,y;T) = F(x,\beta) \tag{I.1}$$

where:

$$x = (x_1, x_2) = (x, y)$$

$$\beta = (\beta_1, \beta_2, \ldots \beta_P)$$

are the model inputs (coordinates in space and time, and aquifer parameters T). Thus the new version of the error criterion equation (3.6) will be:

$$E(x_i;T) \approx \Phi(x_i;T) = \sum_{i=1}^{n} [\, h(x_i;T) - \hat{h}(x_i) \,]^2 \tag{I.2}$$

Where i = 1,2, ... , n denotes the ith observation point and n is the total number of output observations. Expressing in terms of p unknown parameters, (I.2) becomes:

$$\Phi_2(\beta) = \sum_{i=1}^{n} [\, h(x_i;T) - \hat{h}(x_i)]^2 \tag{I.3}$$

2) Linearize (I.1) about an initial estimate b^o of parameter vector b, where b is the current estimate for β, as follows:

$$h_i(x_i,b^o+\delta_b) = F(x_i,b^o) + \nabla F'(x_i,b^o)\,\delta_b = F(x_i,b^o) + \sum_{j=1}^{p}\left(\frac{\partial f}{\partial b_j}(x_i,b)_{|b=b^o}\right)\delta_{bj} \qquad (I.4)$$

where δ_{bj} is the correction vector to b, h_i is the linearized aquifer model output, and p is the number of transmissivity parameters. Substituting (I.4) into the objective function (I.3), yields;

$$\Phi_2(b) \approx \Phi(b) = \sum_{i=1}^{n}\left(F(x_i,b) + \sum_{j=1}^{p}\left(\frac{\partial f}{\partial b_j}(x_i,b)_{|b=b^o}\right)\delta_{bj} - \hat{h}(x_i)\right)^2 \qquad (I.5)$$

3) The correction vector δ_b appears linearly in (I.4), and thus the optimal value can be obtained by the standard least squares method, setting $\partial\Phi/\partial\delta_{bj}^{*} = 0$. This yields:

$$A\,\delta_b = g \qquad (I.6)$$

where:

$$A = J^T J$$

$$J = \left(\frac{\partial F_i}{\partial b_j}\right) \quad i = 1, 2, \ldots, n;\ j = 1, 2, \ldots, p$$

$$F_i = F(x_i,b)$$

$$g_i = \sum_{i=1}^{n} [\hat{h}(x_i) - F_i] \frac{\partial F_i}{\partial b_j} \quad i = 1, 2, \ldots, n; j = 1, 2, \ldots, p$$

4) Scale matrix A and the vector g_S as follows:

$$S = s_{ij} = \frac{a_{ij}}{\sqrt{a_{ii}}\sqrt{a_{jj}}} \tag{I.7}$$

$$g_{Sj} = \frac{g_j}{\sqrt{a_{jj}}} \tag{I.8}$$

5) Apply the Marquardt's modification (3.22) and (3.23), as defined in chapter 3, in an iterative fashion with current step k:

$$[\, S^{(k)} + \mu^{(k)} I \,]\, \delta_b^{(k)} = g_s^{(k)} \tag{I.9}$$

where $\mu^{(k)}$ is chosen such that $\Phi(\, b^{(k+1)}) < \Phi(\, b^{(k)})$

6) Cooley and Naff [1985] suggest the following procedure to compute $\mu^{(k)}$:

Set $\mu^{(0)} = 0$ at the beginning of the regression, then, at each iteration (k) check and recompute μ as necessary using the following formulas:

$$\mu^{(k)} = \mu^{(\ell)} \qquad \text{if } \delta_b^{(k+1)\,T} g_s^{(k)} \geq \cos\theta_{mx} \sqrt{\delta_b^{(k+1)\,T} \delta_b^{(k+1)} \left(g_s^{(k)\,T} g_s^{(k)} \right)} \tag{I.10a}$$

$$\mu^{(k)} = \tfrac{3}{2}\mu^{(\ell)} + C \qquad \text{if } \delta_b^{(k+1)\,T} g_s^{(k)} < \cos\theta_{mx} \sqrt{\delta_b^{(k+1)\,T} \delta_b^{(k+1)} \left(g_s^{(k)\,T} g_s^{(k)} \right)} \tag{I.10b}$$

where $C > 0$, $\theta_{mx} < 90^o$ and ^{T} denotes the transpose of the vector. At the beginning of iteration (k), set $\ell = 1$ and $g_s^{(\ell)} = g_s^{(k-1)}$. Then, (I.9) is solved and (I.10a) or (I.10b) is applied. If equation I.10b is employed, (I.9) is resolved using $\mu^{(\ell+1)}$, and ℓ is incremented by one. This process is repeated until (I.10a) is used, at which point the appropriate value of μ for iteration (k) has been found. This procedure to compute $\mu^{(k)}$ is empirical but has proven to yield values of μ within an acceptable practical range. For θ_{mx}, Cooley suggests a value $< 90^o$.

7) Cooley proposes the following formulas to compute the parameter $\rho^{(k)}$:

$$t^{(k)} = \max_i | \delta_{bi}^{(k+1)} | \tag{I.11}$$

$$\begin{cases} \rho^{(k)} = 1 & \text{if} \quad t^{(k)} \le t_{mx} \\ \rho^{(k)} = \dfrac{t_{mx}}{t^{(k)}} & \text{if} \quad t^{(k)} > t_{mx} \end{cases} \tag{I.12}$$

In (I.12), t_{mx} is the maximum fractional change that any of the parameters can possibly decrease or increase at any iteration and whose optimum value should be obtained by trial and error.

8) Equation (I.6) is solved for $\delta_b^{(k)}$, yielding a new trial vector of parameters $b^{(k)}$:

$$b^{(k+1)} = b^{(k)} + \rho^{(k)} \delta_b^{(k)} \tag{I.13}$$

which in turn leads to a new sum of squares $\Phi(b^{(k+1)})$.

9) Check a stopping criterion to accept convergence such as:

$$\frac{\delta_j^{(k)}}{\tau + | b_j^{(k)} |} < \varepsilon \quad \text{for all j and } \varepsilon > 0 \tag{I.14}$$

Marquardt [1963] suggests values of $\varepsilon = 10^{-5}$ and $\tau = 10^{-3}$.

APPENDIX II

ONE-DIMENSIONAL AQUIFER TEST OF ALGORITHMS

This appendix illustrates the application of the numerical techniques explained in chapters 3 and 4 for the identification of aquifer transmissivities under steady state flow conditions. This numerical evaluation is carried out in two parts. First, the finite element method is evaluated for the solution of hydraulic heads (forward solution) and the solution of the sensitivity coefficients in a simple one-dimensional hypothetical aquifer with known analytical solutions. The second part of this evaluation, consists in the application of the modified Marquardt method of functional minimization and parameter zonation techniques of Chapter 3 and 4 for identification of transmissivities in the one-dimensional aquifer of part 1.

One-Dimensional Steady State Synthetic Model

Let us consider the a one-dimensional aquifer with two transmissivity zones as shown in Figure II.1. The one-dimensional, steady state form of the groundwater flow equation for such an aquifer reduces to:

$$\frac{\partial^2 h}{\partial x^2} + \frac{R}{T} = 0 \qquad \text{(II.1)}$$

where h is the hydraulic head potential, x is the spatial coordinate, R is the zonal rate of recharge and T the zonal transmissivity. The dimensions of h, R and T are (L), (L^3/T) and (L^2/T) respectively. This aquifer is subject to a constant rate of recharge, R_1 and R_2, of 1/20 in zone 1 and of 3/40 in zone 2, uniformly distributed over each zone. Transmissivity values are 10 and 5 for zones 1 and 2, respectively, and the length of each zone is 1 unit.

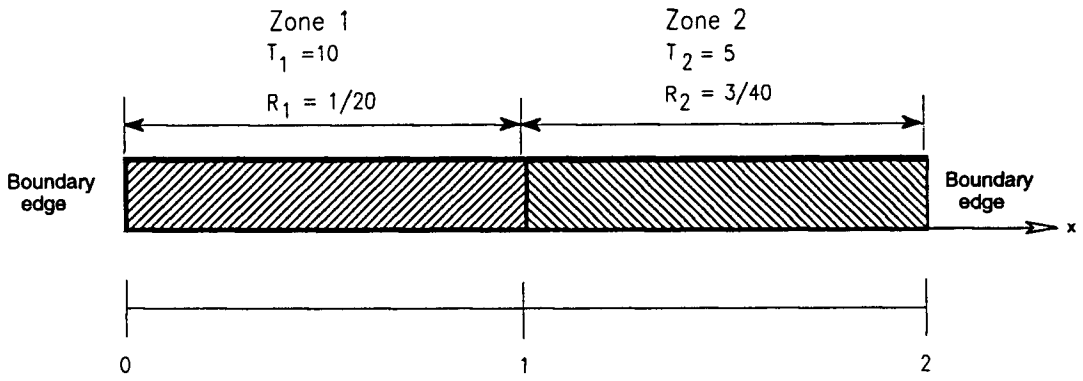

Figure II.1 - One-dimensional hypothetical aquifer with two homogeneous zones

In this example, there are two combinations of boundary conditions of particular interest. It is well known that the type of boundary condition plays an important role in any identification problem, particularly in the indirect approach where a sensitivity matrix is computed from sensitivity coefficients. The first case illustrates the one-dimensional aquifer with constant head specified at both ends and in the second case the aquifer is subject to constant head at one end and flux specified at the other end.

Case 1 - Constant head specified at x = 0 and x = L

Figure II.2 shows the one-dimensional aquifer with head specified at both end. The analytical solution of equation II.1 for the head distribution of the one-dimensional aquifer in this case is:

$$h(x)=\begin{cases}-\dfrac{R_1}{2T_1}x^2+f\,x+H_0 & 0\le x\le 1\\[2ex] -\dfrac{R_2}{2T_2}(x^2-L^2)+\left(\dfrac{R_2-R_1}{T_2}+\dfrac{T_1}{T_2}f\right)(x-L)+H_L & 1\le x\le L\end{cases} \qquad \text{(II.2)}$$

Where:

$$f=\frac{1}{2(T_1+T_2)}\left(2T_2(H_L-H_o)+R_1\frac{T_2}{T_1}+2R_1+R_2\right)$$

R_1 = Recharge in zone 1

R_2 = Recharge in zone 2

T_1 = Transmissivity in zone 1

T_2 = Transmissivity in zone 2

H_L = Constant head at x = L

H_O = Constant head at x = 0

L = Length of aquifer

h(x) = hydraulic head

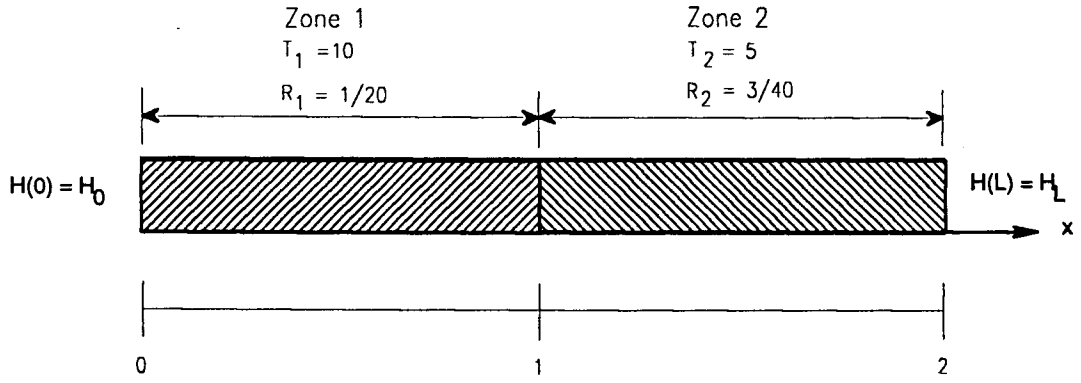

Figure II.2 - One-dimensional hypothetical aquifer with two homogeneous zones and constant head specified at both ends (Case 1)

The analytical expressions for the sensitivity coefficients, U_{T1} and U_{T2} are as follows:

$$U_{T_1} = \frac{\partial h}{\partial T_1} = \begin{cases} \dfrac{R_1 x^2}{2T_1^2} + \dfrac{\partial f}{\partial T_1} & 0 \le x \le 1 \\ \dfrac{f}{T_2}(x-L) + \dfrac{T_1}{T_2}\dfrac{\partial f}{\partial T_1}(x-L) & 1 \le x \le L \end{cases} \tag{II.3}$$

$$U_{T_2} = \frac{\partial h}{\partial T_2} = \begin{cases} \dfrac{\partial f}{\partial T_2} x & 0 \le x \le 1 \\ \dfrac{R_2}{2T_2}(x^2 - L^2) - \dfrac{R_2 - R_1}{T_2^2} - \dfrac{T_1}{T_2^2} f(x-L) + \dfrac{T_1}{T_2}\dfrac{\partial f}{\partial T_2}(x-L) & 1 \le x \le L \end{cases} \tag{II.4}$$

where:

$$\frac{\partial f}{\partial T_1} = \frac{T_2}{T_1 + T_2}\left(-\frac{f}{T_2^2} - \frac{R_1}{2T_1^2}\right)$$

and

$$\frac{\partial f}{\partial T_2} = \frac{T_2}{T_1 + T_2}\left(\frac{2T_1 f - R_2 - 2R_1}{2T_2^2}\right)$$

In this example, if we make $H_L = 149/50$, $H_O = 0$, T1 = 10, T2 = 5, L = 2, R1 = 1/20 and R2 = 3/40, then f = 1, $\partial f/\partial T_1 = -801/12000$, $\partial f/\partial T_2 = 793/6000$, and the equations II.2 to II.4 for the head and sensitivity coefficients become:

$$h(x) = \begin{cases} -\frac{x^2}{400} + x & 0 \le x \le 1 \\ -\frac{3x^2}{400} + \frac{401x}{200} - 1 & 1 \le x \le 2 \end{cases} \qquad \text{(II.5)}$$

$$U_{T1} = \frac{\partial h}{\partial T_1} = \begin{cases} \frac{x^2}{4000} - \frac{801x}{12000} & 0 \le x \le 1 \\ \frac{399x}{6000} - \frac{399}{3000} & 1 \le x \le 2 \end{cases} \qquad \text{(II.6)}$$

$$U_{T2} = \frac{\partial h}{\partial T_2} = \begin{cases} \frac{793x}{6000} & 0 \le x \le 1 \\ \frac{3x^2}{2000} - \frac{41x}{300} + \frac{401}{1500} & 1 \le x \le 2 \end{cases} \qquad \text{(II.7)}$$

Case 2. Constant head specified at x = 0 and flux specified at x = L

The second aquifer configuration of interest consists of the same aquifer as in Case 1 but with constant head H specified at x = 0 and flux Q specified at x = L as shown in Figure II.3. The analytical solution for the head distribution and the sensitivity coefficients are given by the following expressions:

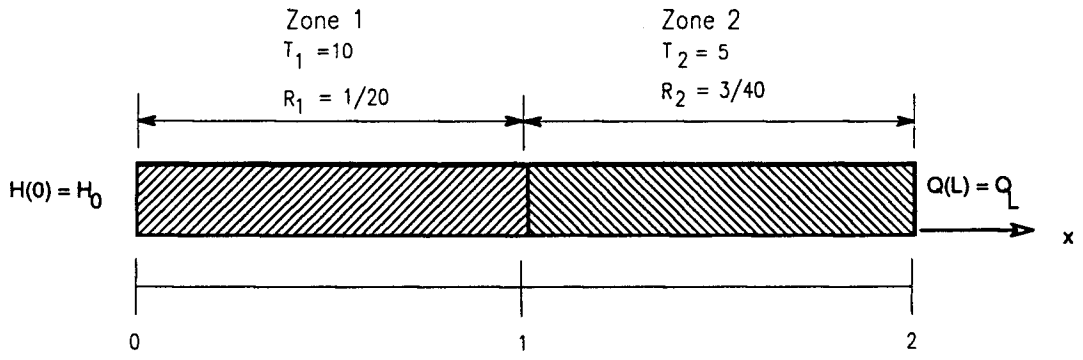

Figure II.3 - One-dimensional hypothetical aquifer with two homogeneous zones and constant head H specified at x = 0 and Q at x = L (Case 2)

$$h(x)=\begin{cases} -\dfrac{R_1x^2}{2T_1}+\dfrac{Q_L+R_2(3-L)+R_1}{T_1}+H_o & 0\le x\le 1 \\ -\dfrac{R_2x^2}{2T_2}+\dfrac{Q_L+2R_2x}{T_2}+H_o-\dfrac{2Q_L+3R_2}{2T_2}+\dfrac{2Q_L+2R_2(3-L)+R_1}{2T_1} & 1\le x\le L \end{cases} \qquad \text{(II.8)}$$

The sensitivity coefficients, U_{T1} and U_{T2} are given by:

$$U_{T_1} = \frac{\partial h}{\partial T_1} = \begin{cases} \dfrac{R_1 x^2 - 2x[Q_L + R_2(3-L) + R_1]}{2T_1^2} & 0 \le x \le 1 \\ -\dfrac{2Q_L + 2R_2(3-L) + R_1}{2T_1^2} & 1 \le x \le L \end{cases} \qquad \text{(II.9)}$$

$$U_{T_2} = \frac{\partial h}{\partial T_2} = \begin{cases} 0 & 0 \le x \le 1 \\ \dfrac{R_2 x^2}{2T_2} - \dfrac{(Q_L + 2R_2)x}{T_2^2} + \dfrac{2Q_L + 3R_2}{2T_2^2} & 1 \le x \le L \end{cases} \qquad \text{(II.10)}$$

If $Q_L = 711/72$, $H_O = 0$, $T_1 = 10$, $T_2 = 5$, $L = 2$, $R_1 = 1/20$ and $R_2 = 3/40$ then equations II.8 to II.10 become:

$$h(x) = \begin{cases} -\dfrac{x^2}{400} + x & 0 \le x \le 1 \\ -\dfrac{3x^2}{4000} + \dfrac{401x}{200} - 1 & 1 \le x \le 2 \end{cases} \qquad \text{(II.11)}$$

$$U_{T1} = \frac{\partial h}{\partial T_1} = \begin{cases} \dfrac{x^2}{4000} - \dfrac{x}{10} & 0 \le x \le 1 \\ -\dfrac{399}{4000} & 1 \le x \le 2 \end{cases} \qquad \text{(II.12)}$$

$$U_{T2} = \frac{\partial h}{\partial T_2} = \begin{cases} 0 & 0 \le x \le 1 \\ \dfrac{3x^2}{2000} - \dfrac{401x}{1000} + \dfrac{799}{2000} & 1 \le x \le 2 \end{cases} \qquad \text{(II.13)}$$

The application of the finite element method to solve equation II.1 for the two-zoned aquifer, requires the discretization of the domain into finite elements. In order to evaluate the accuracy of the finite element method when solving for the heads and the sensitivity coefficients, the numerical solutions were compared to the analytical results. Domain discretizations using a different number of finite elements, ranging from two to twenty were used to verify the adequacy of the quadratic interpolation function used to approximate the solution over each element. In all cases the finite element solution compared favorably to the analytical solution. Figure II.4 compares the head distribution resulting from a 20 element discretization to the analytical solution given by equations II.11. Likewise, the computed sensitivity coefficients of the heads with respect to each of the transmissivity zones were also compared with their corresponding analytical solutions given by equations II.6 and II.7 for the case of constant head at both ends (Fig. II.5), and by equations II.12 and II.13 for the case of head specified at $x = 0$ and flux specified at $x = 2$ (Fig. II.6). For both cases of boundary conditions, the resulting finite element solutions for the head and sensitivity coefficients closely matches the correspondent analytical solution.

Least Squares Solution for Transmissivities

The nonlinear regression procedure based on Marquardt's algorithm was verified by identifying the transmissivities for the two-zone aquifer T_1 and T_2. For this example, the two-zone aquifer was divided into two zones using four quadrilateral finite elements of equal size as shown in Figures II.7 and II.8. There are four head observation locations at $x = 0.5$, 1.0, 1.5 and 2.0 where noiseless data is available.

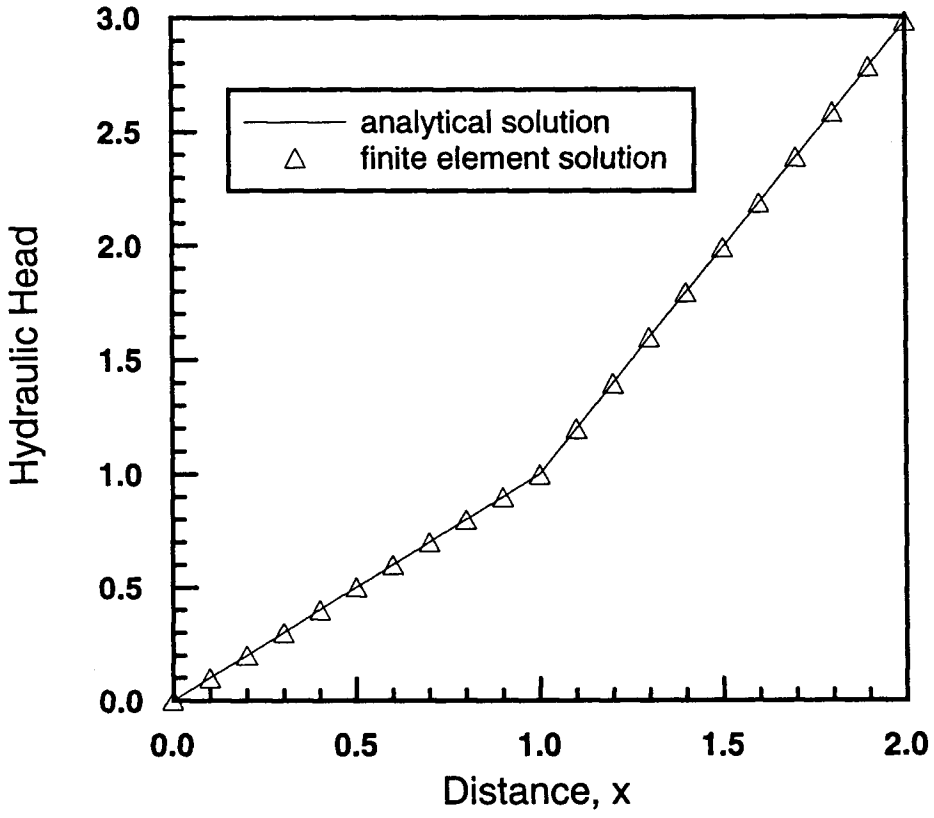

Figure II.4 - Analytical and Finite Element Solution for Head Distribution in 1-D, 2-zone Aquifer.

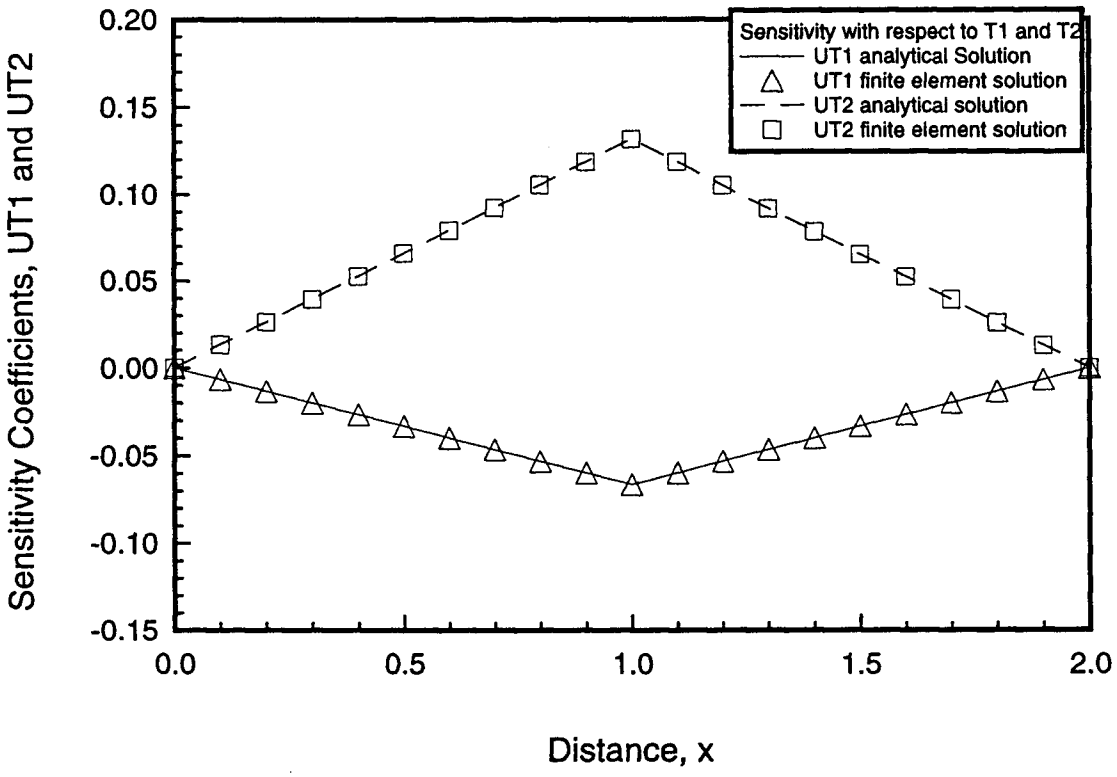

Figure II.5 - Analytical and Finite Element Solution for Sensitivity Coefficients With Respect to T1 and T2. Case 1 - Head Specified at Both Ends of the Aquifer.

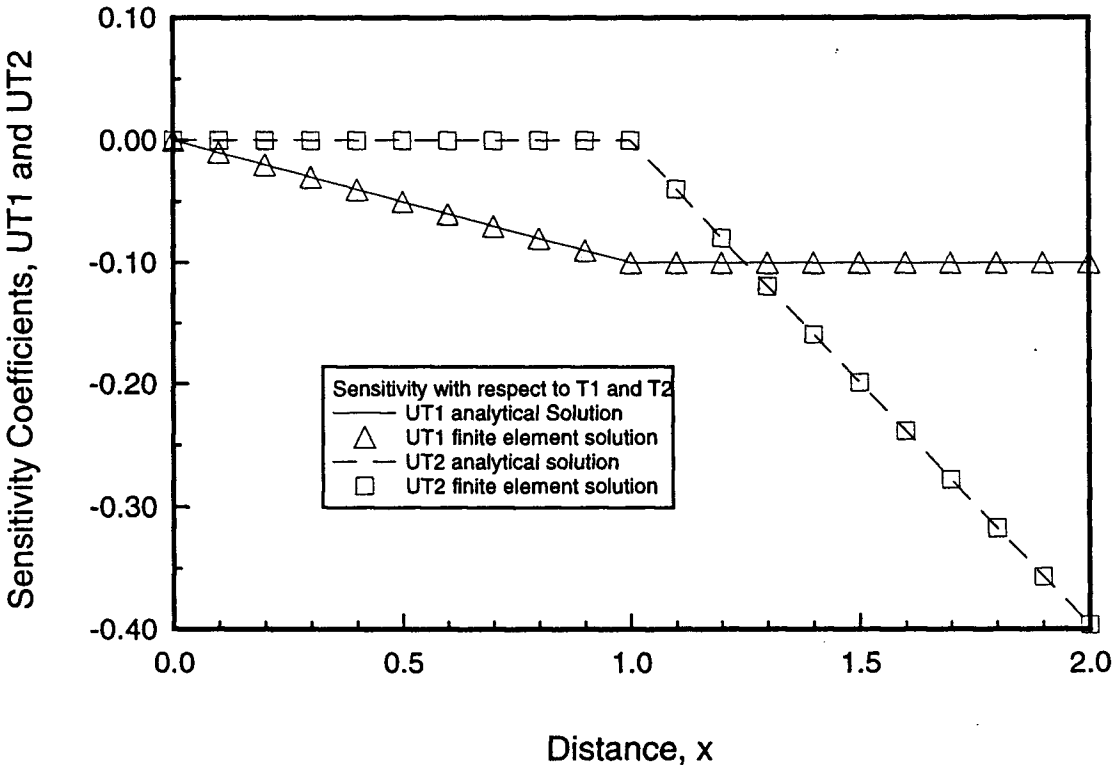

Figure II.6 - Analytical and Finite Element Solution for Sensitivity Coefficients With Respect to T1 and T2. Case 2 - Head Specified at x = 0 and Q Specified at x=2.

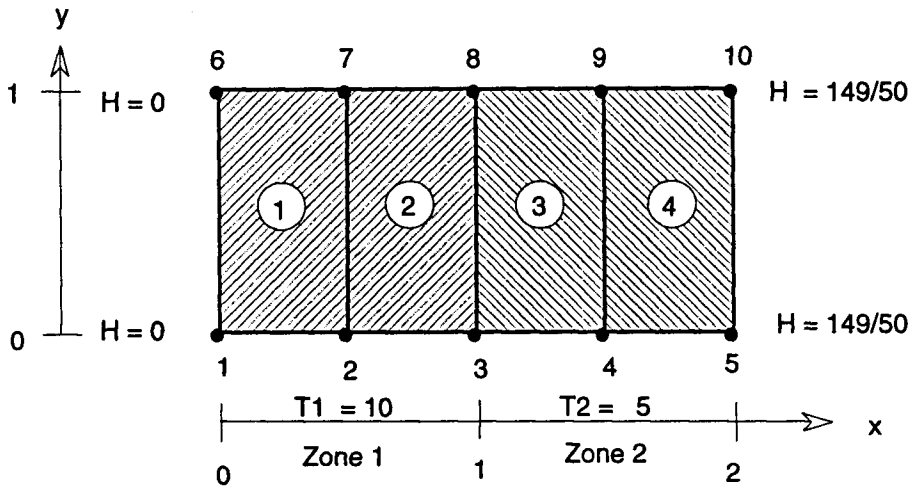

Figure II.7. Finite element discretization of 1-dimensional aquifer with two transmissivity zones. Head specified at x = 0 and x = 2

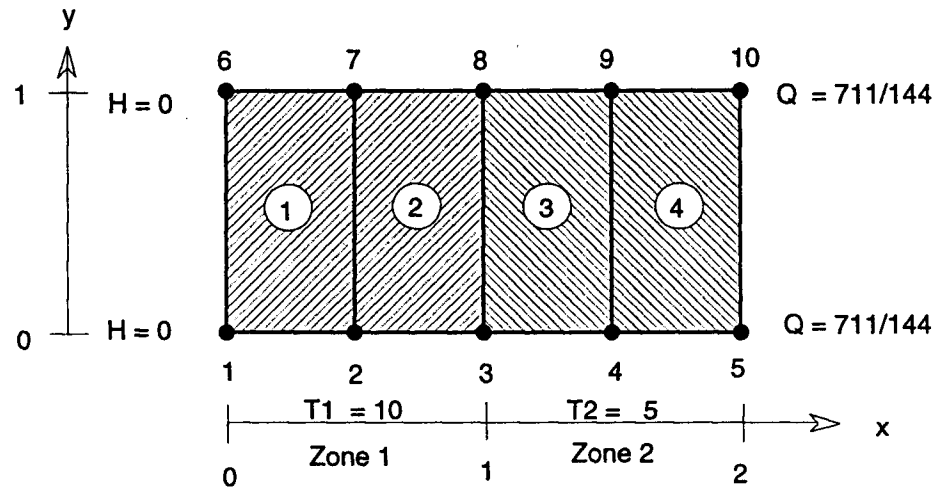

Figure II.8. Finite element discretization of 1-dimensional aquifer with two transmissivity zones. Head specified at x = 0 and flux specified at x = 2

The known head distribution is given by equation II.11 and is used to assign head values at the observation points. Two initial sets of transmissivity values were used as initial transmissivity vectors for T1 and T2 of (1.0,1.0) and (100,100). The maximum allowable change in the correction vector at any iteration was set at 5 for both cases. The results of the minimization of the objective function for both types of boundary conditions are summarized in Tables II.1 and II.2.

Table II.1 - Statistical Results for Identification Problem.
Case 1-Constant Head at Both Ends

Initial T		No. of	Computed T		Final	Computed	Standard Error	
Zone 1	Zone 2	Iterations	T1	T2	Φ	Variance	Zone 1	Zone 2
1.0	1.0	6	9.999998	4.999999	3.2334E-12	8.0835E-15	6.1018E-4	3.0759E-4
100.0	100.0	21	9.999998	4.999999	1.1569E-10	2.8923E-10	3.6499E-3	1.8399E-3

Table II.2 - Statistical Results for Identification Problem.
Case 2-Constant Head at x = 0 and Q at x = 2

Initial T		No. of	Computed T		Final	Computed	Standard Error	
Zone 1	Zone 2	Iterations	T1	T2	Φ	Variance	Zone 1	Zone 2
1.0	1.0	7	10.0000	5.000000	5.3274E-11	1.3319E-12	3.3421E-6	1.5937E-6
100.0	100.0	24	10.0000	5.000000	1.1569E-10	2.7277E-10	1.5124E-4	7.2116E-5

The values of the objective function for each case are illustrated in Figures II.9 and II.10. For Case 1, where constant head is specified at both ends of the aquifer, it is clear that the solution is non-unique. The solution lies along the line $\phi = 0$ and it depends on the location of the initial value (T_1^0, T_2^0). The imposition of constraints on the parameters in the Marquardt algorithm an the use of more information points than unknown parameters lead to convergence to the exact values.

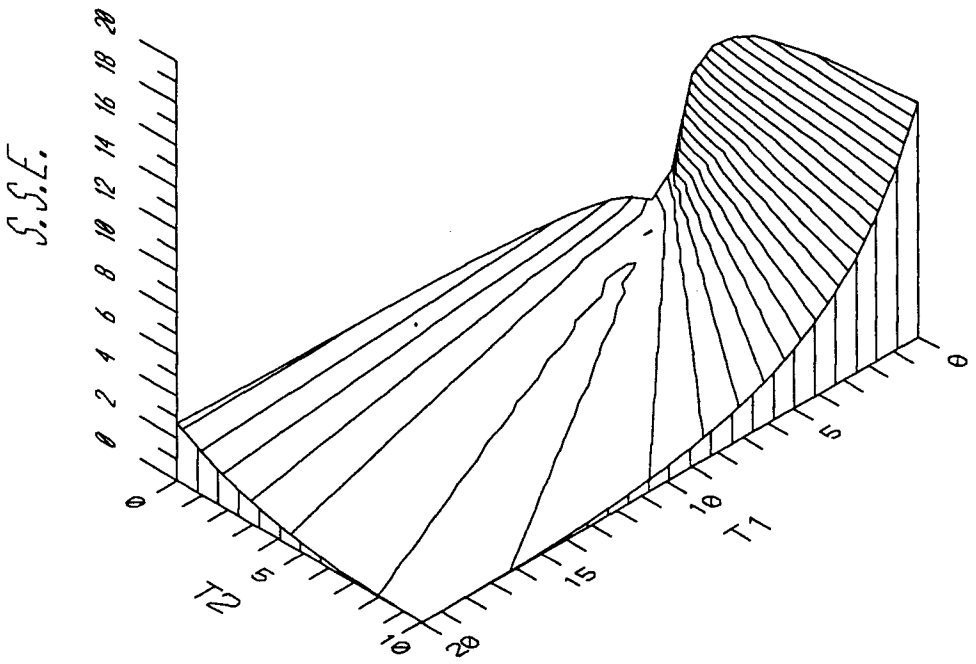

Figure II.9 - Objective Function for Case 1. Constant Head Specified at x = 0 and x = 2

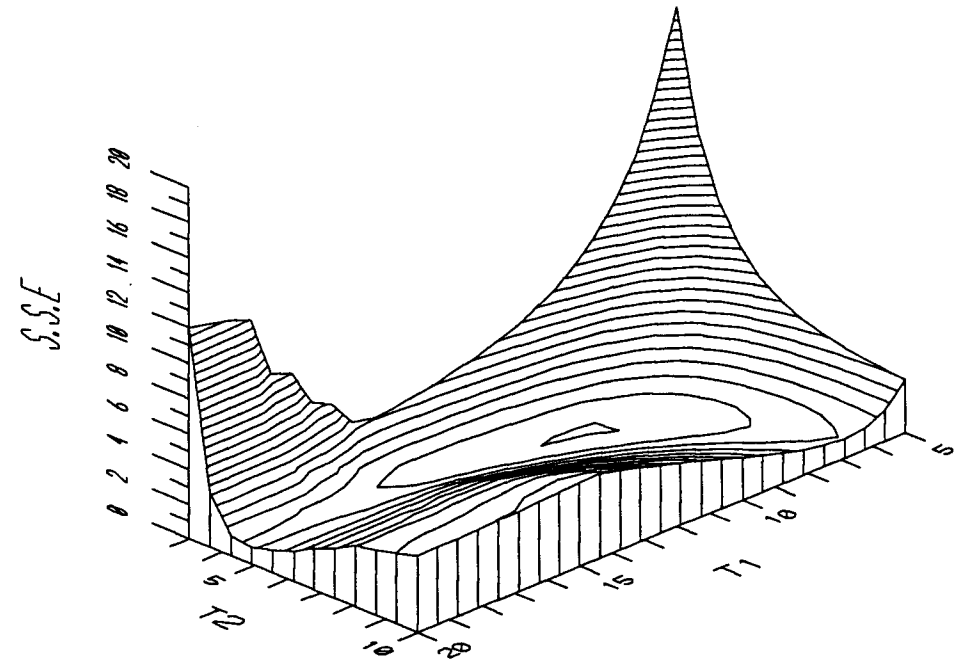

Figure II.10 - Objective Function for Case 2. Constant Head Specified at x = 0 and Flux at x = 2

In case 2, the specification of flux at the right boundary, Q(L=2), has increased the overall sensitivity of the system resulting in more accurate estimates. As Figure II.10 shows, the objective function is convex all around the solution $\Phi(T_1, T_2) = 0$ at $T_1 = 10$ and $T_2 = 5$. In the neighborhood of the solution the convexity of the function is obvious. However, as one approaches the solution, there is a considerable decrease in the rate of convergence due to the flattening of the function near the solution.

Parameterization by Zonation

To illustrate the parameterization procedure, we will induce ill-conditioning to the previous one-dimensional aquifer by further subdividing it into 4 equal zones (Figure II.7). Theoretically, in any identification problem, there must be at least n observations or more to identify n parameters and n + 1 observations to compute error estimates for the identified parameters based on their covariances. In this example with four observation points and four parameters, we should expect some degree of ill-conditioning from the point of view of least squares because of the location of the observation points. In this case, the given observation points do not provide sufficient information to identify all four parameters. This is often the case in real life problems where $n \geq p$ because, in many instances, the observed data at certain locations do not provide information about all the parameters.

Case 1 - Constant head speficied at both ends

Under these boundary conditions, the identification of the four zonal transmissivities started with the initial values all equal to unity. The history of values of the parameters and the objective function, Φ, is shown in Table II.3. After 2 iterations, the value of the parameter T3 has become negative pulling away from the solution. This sudden change in the value of the objective function could be an

indication of instability. At this point it is convenient to test for the presence of ill-defined parameters in the solution using the singular value decomposition of the design matrix A. At this iteration the upper triangular portion of the symmetric design matrix A is:

$$A = \begin{pmatrix} .474996 & .102767 & -.051736 & -.704762 \\ & .218642 & -.009234 & -.441758 \\ & & .026064 & .024289 \\ & & & 1.594976 \end{pmatrix}$$

The singular value decomposition of the design matrix A can be expressed as:

$$A = U\,W\,V^T$$

where:

$$U = \begin{pmatrix} .3012 & -.7454 & .4291 & .4115 \\ .6047 & .6246 & .4339 & .2363 \\ -.6642 & .1416 & .7337 & -.0223 \\ .3201 & -.1845 & .2986 & -.8799 \end{pmatrix}$$

$$W = \begin{pmatrix} 2.04379 & & & \\ & 0.22429 & & \\ & & 5.59083E-17 & \\ & & & 0.00466 \end{pmatrix}$$

$$V^T = U^T \qquad G = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The singular value decomposition of the design matrix A points at the parameter T3 as the prime candidate for elimination ($w_3 \approx 0$ in matrix W). Since zone 3 is surrounded by two other zones (T2 and T4), there are two possible three-parameter models that can be obtained from combining T3 with each adjacent zone. The first three-parameter model obtained after combining T2 with T3 lead to a reduced value of the objective function Φ' equal to 0.327324 and a new value of the determinant of the design matrix, Det A, equal to 0.001274. The second model obtained from combining T4 and T3 also leads to a smaller value of the objective function Φ' equal to 0.012035 and Det A equal to 0.009204.

Table II.3. Values of Estimated Transmissivities and Φ During Least Squares Minimization for Case 1.

	Parameter Value				Objective Function
Iteration	**T1**	**T2**	**T3**	**T4**	**Φ**
0	1.000	1.000	1.000	1.000	0.83687
1	1.500	1.500	2.500	1.000	0.59228
2	1.500	2.000	-1.500	0.750	5.08813
Parameterization after 2 iterations Parameter T3 eliminated from solution. New Zone 4 = Zone 3 $\cup$ Zone 4					
3	1.5	2.000		0.750	0.01203
4	2.775	3.074		1.388	0.00151
5	4.780	4.970		2.390	2.2215E-04
6	7.275	7.369		3.634	2.36897E-05
7	9.257	9.282		4.629	1.01185E-06
8	9.945	9.947		4.972	4.53923E-09
9	9.999	9.999		4.999	1.28468E-13
10	10.000	10.000		5.000	1.11947E-22

Each reduced parameter model significantly improves the current value of the objective function over the four-parameter problem. It is obvious that the combination of T3 and T4 yields the most sensitive model and the smallest value of the objective function. Accepting the combination of T3 and T4 as the best pattern, we restart the minimization at this point by computing the parameter correction vector as given by equation 4.23:

$$\delta_t' = [\ 1.27500 \quad 1.07154 \quad 0.63750\ ]^T$$

The new vector of model parameters given by equation 4.24 is:

$$\mathbf{T} = G'' T + \delta_t' = [\ 5.942 \quad 6.818 \quad 4.651\ ]^T$$

This reduced set of parameters leads to the exact solution after eight additional iterations (see Table II.3). For the four-parameter model with four observations, the covariance matrix is not defined since n equals p. Therefore, an approximation to the covariance matrix was obtained for both the four and three-parameter models by assuming that n-p equals to one for both cases. The upper triangular portion of the symmetric covariance matrices for the four and three-parameter models are:

$$P_{4x4} = \begin{pmatrix} 9.5467E+08 & 9.6550E+08 & 1.6323E-09 & 6.6439E+08 \\ & 9.7645E+08 & 1.6508E+09 & 6.7193E+08 \\ & & 2.7909E+09 & 1.1360E+09 \\ & & & 4.6237E+08 \end{pmatrix}$$

$$P_{3x3} = \begin{pmatrix} 4.4955E-07 & 4.4999E-07 & 2.2656E-07 \\ & 4.5045E-07 & 2.2978E-07 \\ & & 1.1418E-07 \end{pmatrix}$$

After comparing the covariance matrices for the four and three-parameter models, it is obvious that the deletion of the ill-defined parameter T3 from the solution has a profound effect in reducing the magnitude of the individual variances of the estimated parameters (square root of diagonal elements of the covariance matrix). For the four and three-parameter models the individual variances and standard errors for the identified parameters respectively are:

Var $(b_{LS})_4$ = (9.5467E+08 9.7645E+08 2.7909E+09 4.6237E+08)

Std. Error $(b_{LS})_4$ = (30897.7 31248.2 52828.9 21502.8)

Var $(b_{LS})_3$ = (4.4955E-07 4.5045E-07 1.1418E-07)

Std Error $(b_{LS})_3$ = (6.7048E-04 6.7111E-04 3.3791E-04)

Case 2 - Constant head Specified at x=0 and flux at x=L

A similar numerical experiment to Case 1 was carried out using a fixed value of head H(x=0) and a constant discharge Q(x=2) of 711/72. The identification of the four zonal transmissivities was also started with the initial values all equal to one. The history of values of the parameters and the objective function, Φ, is shown in Table II.4. After only two iterations, the value of the parameter corresponding to zone 4, T4, has become negative. It is obvious that T4 is diverging towards minus infinity and yet the value of the objective function still decreases with each iteration. This is a typical case of model insensitivity due to lack of information provided by the heads

about parameter T4. This problem, as it is posed with four unknowns, does not have a unique solution. It is by the technique of parameter zonation that we seek to eliminate the ill-defined parameter T4 from the solution so that a minimum in the objective function can be found. Since convergence was not achieved after the maximum number of iterations allowed, zonation of the transmissivity zones is then applied to find a coarser parameter zonation pattern which may leads us to the desired minimum in the objective function value.

Table II.4. Values of Estimated Transmissivities and Φ During Least Squares Minimization for Case 2.

	Parameter Value				Objective Function
Iteration	**T1**	**T2**	**T3**	**T4**	**Φ**
0	1.000	1.000	1.000	1.000	536.99433
1	1.900	1.900	1.800	2.000	117.66667
2	2.862	2.862	2.520	-3.000	39.49997
3	4.905	4.905	3.770	-4.591	6.38675
4	7.404	7.404	4.697	-6.407	0.64841
5	9.326	9.326	4.982	-9.313	3.44742E-02
6	9.955	9.955	4.999	-13.438	9.35270E-05
7	9.976	9.976	5.000	-18.438	2.64493E-05
⋮	⋮	⋮	⋮	⋮	⋮
25	10.000	10.000	5.000	-83.438	9.154465E-10
⋮	⋮	⋮	⋮	⋮	⋮
100	10.000	10.000	5.000	-311.1	1.18774E-27
No convergence after 100 Iterations. Parameterization after 100 iterations Parameter T4 eliminated from solution. New Zone 3 = Zone 3 ∪ Zone 4					
101	10.000	10.000	5.000		5.82401E-32

At iteration 100, the elements of the upper portion of the symmetric matrix A are given by:

$$A = \begin{pmatrix} .014962 & .009950 & .019838 & -2.760780E-20 \\ & .000993 & .001979 & -2.353316E-20 \\ & & .007890 & -6.224821E-20 \\ & & & 6.672086E-38 \end{pmatrix}$$

The singular value decomposition of the design matrix A is given by:

$$A = U\,W\,V^T$$

where:

$$U = \begin{pmatrix} -2.7748E-01 & 8.0895E-01 & -5.1831E-01 & -8.0512E-19 \\ -2.6145E-01 & 4.5556E-01 & 8.5095E-01 & -7.8924E-19 \\ -9.2449E-01 & -3.7157E-01 & -8.5128E-02 & -3.8856E-19 \\ 7.8892E-20 & -8.6647E-20 & -2.2122E-20 & -1.0000E-00 \end{pmatrix}$$

$$W = \begin{pmatrix} 9.0452E-02 & & & \\ & 1.1454E-02 & & \\ & & 1.8850E-03 & \\ & & & 1.7327E-40 \end{pmatrix}$$

$$V^T = U^T \qquad G = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

The parameter correction vector as given by (4.23) is:

$$\delta_t' = [\ 4.55761E\text{-}14 \quad 4.55761E\text{-}14 \quad 2.20787E\text{-}14\ ]^T$$

A near zero value of w_4 corresponding to parameter T4 in matrix W indicates that this parameter should be removed from the solution. Using matrix G for such purpose, T4 can now be deleted from the solution. The only possible combination T4 with surrounding zones is with T3. Thus, the new vector of model parameters given by (4.24) is:

$$T = G'' T + \delta_t' = [\ 10.0000 \quad 10.0000 \quad 5.0000\ ]^T$$

The upper triangular portion of the symmetric covariance matrices, P, of the four and three-parameter models are, respectively.

$$P_{4x4} = \begin{pmatrix} 4.1788E\text{-}28 & 1.2052E\text{-}28 & 1.3130E\text{-}28 & 3.3792E\text{-}10 \\ & 5.5452E\text{-}28 & 9.1961E\text{-}29 & 3.3125E\text{-}10 \\ & & 8.1802E\text{-}29 & 1.6308E\text{-}10 \\ & & & 4.1971E\text{-}10 \end{pmatrix}$$

$$P_{3x3} = \begin{pmatrix} 4.0131E\text{-}27 & -4.0232E\text{-}27 & 7.8856E\text{-}43 \\ & 8.0666E\text{-}27 & -1.0115E\text{-}27 \\ & & 5.0734E\text{-}28 \end{pmatrix}$$

This set of three parameters leads to immediate convergence to the exact solution. The measures of parameter reliability, condition number and determinant of the matrix A are also used in this section as reliability indicators for the identified parameters. The value of the condition number and the determinant of the matrix A for the three-parameter model are, respectively, Cond A_{3x3} = 4.79854E+02 and Det A_{3x3} = 1.952936E-05. For the four-parameter model, Det A_{4x4} = 1.303015E-43 and Cond A_{4x4} = 1.355685E+36. It is clearly shown in this example that the four-parameter model leads to a nearly-singular matrix A, as indicated by the small value of the determinant and large condition number of the matrix A. After zonation of the four original transmissivity zones, a reduced three-parameter model was identified which lead to convergence to the exact solution and more reliable parameters.

Finally, the individual variances and standard errors of the identified parameters for the four and three-parameter models are:

Var $(b_{LS})_4$ = (4.1788E-28 5.5452E-27 8.1802E-29 4.1971E-10)

Std. Error $(b_{LS})_4$ = (2.0442E-14 7.4466E-14 9.0444E-15 2.0486E-05)

Var $(b_{LS})_3$ = (4.0131E-27 8.0667E-27 5.0734E-28)

Std Error $(b_{LS})_3$ = (6.3349E-14 8.9815E-14 2.2524E-14)

It is clear in this example that the problem is not accuracy in the identified parameters between the four and three-parameter models but convergence due to lack of information to identify T4 in the original four parameter model.

From the numerical examples presented herein, we can conclude that the type of boundary conditions significantly affect the overall sensitivity of a model. Equally important in any groundwater parameter identification problem is the amount of

informative head data available. Under noiseless head data conditions, the proposed methods of parameter zonation of Chapters 3 and 4 were successfully applied for the identification of the zonal transmissivities of a simple one-dimensional aquifer.