

Review of Parameter Identification Procedures in Groundwater Hydrology: The Inverse Problem

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The purpose of this survey is to review parameter identification procedures in groundwater hydrology and to examine computational techniques which have been developed to solve the inverse problem. Parameter identification methods are classified under the error criterion used in the formulation of the inverse problem. The problem of ill-posedness in connection with the inverse problem is addressed. Typical inverse solution techniques are highlighted. The review also includes the evaluation of methods used for computing the sensitivity matrix. Statistics which can be used to estimate the parameter uncertainty are outlined. Attempts have been made to compare and contrast representative inverse procedures, and direction for future research is suggested.

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INTRODUCTION

In recent years, simulation and mathematical models have often been used to analyze a groundwater system. In general, physically based mathematical models are solved by finite-difference or finite-element approximations. Most of the groundwater models are distributed parameter models, and the parameters used in deriving the governing equation are not directly measurable from the physical point of view and have to be determined from historical observations. Traditionally, the determination of aquifer parameters is based upon trial-and-error and graphical matching techniques under the assumptions that the aquifer is homogeneous and isotropic and a closed-form solution for the governing equation exists [Theis, 1935]. Such techniques would be inapplicable in a situation where aquifer parameters vary with space or no closed-form solution exists for the governing equation.

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The problem of parameter identification in distributed parameter systems has been studied extensively during the last two decades. The term "distributed parameter system" implies that the response of the system is governed by a partial differential equation and parameters imbedded in the equation are spatially dependent. The inverse problem of parameter identification concerns the optimal determination of the parameters by observing the dependent variable collected in the spatial and time domains. The number of observations is finite and limited, whereas the spatial domain is continuous. For an inhomogeneous aquifer the dimension of the parameter is theoretically infinite. In practice, spatial variables are approximated by a finite-difference or finite-element scheme while the aquifer system is subdivided into several subregions with each subregion characterized by a constant parameter. The reduction of the number of parameters from the infinite dimension to a finite dimensional form is called parameterization.

There are two types of errors associated with the inverse problem: (1) the system modeling error, as represented by a performance criterion, and (2) the error associated with parameter uncertainty. An increase in parameter dimension (the number of unknown parameters associated with parameterization) will generally improve the system modeling error, but will increase the parameter uncertainty and vice versa. The optimum level of parameterization depends on the quantity and quality of data (observations).

ILL-POSEDNESS

The inverse problem is often ill-posed. The ill-posedness is generally characterized by the nonuniqueness and instability of the identified parameters. The instability of the inverse solution stems from the fact that small errors in heads will cause serious errors in the identified parameters.

Chavent [1974] studied the uniqueness problem in connection with parameter identification in distributed parameter systems. As was pointed by Chavent, the uniqueness problem has a great practical importance, because in the case of nonuniqueness, the identified parameters will differ according to the initial estimate of the parameters, and there will be no reason for the estimated parameters to be close to the "true" parameters. As a consequence, the responses of model and system may differ for inputs different from those that have been used for identification. Chavent studied the uniqueness problem for two situations: (1) the case of constant parameters and (2) the case of distributed parameters in space. In case 1, i.e., constant parameters, there are generally more measurements than unknowns, so that the general situation is that the

inverse problem is unique. In case 2, i.e., distributed parameters, if only point measurements are available, the inverse problem is always nonunique. The term, point measurements refers to the situation where measurements are made only at a limited number of locations in the spatial domain.

The uniqueness problem in parameter identification is intimately related to identifiability. The notion of identifiability addresses the question of whether it is all possible to obtain unique solutions of the inverse problem for unknown parameters of interest in a mathematical model, from data collected in the spatial and time domains. Kitamura and Nakagiri [1977] formulated the parameter identification problem as the one-to-one property of the inverse problem, i.e., the one-to-one property of mapping from the space of system outputs to the space of parameters. However, the uniqueness of such a mapping is extremely difficult to establish and often nonexistent. They defined the identifiability as follows: "We shall call an unknown parameter "identifiable" if it can be determined uniquely in all points of its domain by using the input-output relation of the system and the input-output data." Kitamura and Nakagiri also obtained some results for parameter identifiability or nonidentifiability for a system characterized by a linear, one-dimensional parabolic partial differential equation.

Another definition of identifiability was given by Chavent [1979b], which is suited to the identification process using the output least square error criterion. If such criterion is used for solving the inverse problem of parameter identification, the parameter is said to be output least square identifiable if and only if a unique solution of the optimization problem exists and the solution depends continuously on observations. Chavent [1983] presented a weaker sufficient condition for output least square identification.

Identifiability is usually not achievable in the case of point measurements where data is only available at a limited number of locations in the spatial domain. In view of the various uncertainties involved in groundwater modeling, a groundwater model can only be used to approximate the behavior of an aquifer system. If a small, prescribed error is allowed in prediction, Yeh and Sun [1984] developed an extended identifiability criterion which can be used for designing an optimum pumping test to assist parameter identification. The extended identifiability is called the " δ identifiability," which is based on the concept of weak uniqueness.

CLASSIFICATION OF PARAMETER IDENTIFICATION METHODS

Various techniques have been developed to solve the inverse problem of parameter identification. Neuman [1973] classified the techniques into either "direct" or "indirect." The "direct approach" treats the model parameters as dependent variables in a formal inverse boundary value problem. The "indirect approach" is based upon an output error criterion where an existing estimate of the parameters is iteratively improved until the model response is sufficiently close to that of the measured output. In a survey paper by Kubrusly [1977] on distributed parameter systems identification, he classified the identification procedures into three categories: (1) direct method, which consists of those methods that use optimization techniques directly to the distributed (infinite-dimensional) model; (2) reduction to a lumped parameter system, which consists of those methods that reduce the distributed parameter system to a continuous or discrete-time lumped parameter system which is described by ordinary differential equation or difference equation; and (3) reduction to an algebraic equation, which consists of those methods that reduce the partial differential equation to an algebraic equation.

There are only two types of error criteria that have been used in the past in the formulation of the inverse problem for a distributed parameter system. Chavent [1979b] classified the identification procedures into two distinctive categories based upon the error criterion used in the formulation. His classification is intrinsically consistent with Neuman's [1973]. Hence we shall classify the inverse solution methods into the following two categories based upon the error criterion used in the formulation of the inverse problem.

Equation Error Criterion (Direct Method as Classified by Neuman)

If head variations and derivatives (usually estimated) are known over the entire flow region and if the measurement and model errors are negligible, the original governing equation becomes a linear first-order partial differential equation of the hyperbolic type in terms of the unknown parameters. With the aid of boundary conditions and flow data, a direct solution for the unknown parameters may be possible.

In practice, observation wells are sparsely distributed in the flow region in an arbitrary fashion and only a limited number of observation wells are available. To formulate the inverse problem by the equation error criterion, missing data (observations) have to be estimated by interpolation. The interpolated data contain errors in interpolation. If the interpolated data along with observations, which also contain noise, are substituted into the governing equation, an error term will result. Such an error is called the equation error. The error is then minimized over the proper choice of parameters. It should be noted that approximating head variations in the entire domain using an interpolation scheme, without considering the statistical properties of sampling, would cause errors in the results of parameter identification.

Among the available techniques we may mention the energy dissipation method [Nelson, 1968]; linear programming [Kleinecke, 1971]; the use of a flatness criterion [Emsellem and de Marsily, 1971]; the multiple-objective decision process [Neuman, 1973]; the Galerkin method [Frind and Pinder, 1973]; the algebraic approach [Sagar et al., 1975]; the inductive method [Nutbrown, 1975]; linear programming and quadratic programming [Hefez, 1975]; minimization of a quadratic objective function with penalty function [Navarro, 1977]; and the matrix inversion method allied with kriging [Yeh et al., 1983]. To minimize the instability and nonuniqueness, regularity conditions are often required. Table 1 presents some typical parameter identification models that are based upon the equation error criterion.

Output Error Criterion (Indirect Method as Classified by Neuman)

The criterion used in this approach is generally the minimization of a "norm" of the difference between observed and calculated heads at specified observation points. The main advantage of this approach is that the formulation of the inverse problem is applicable to the situation where the number of observations is limited, and it does not require differentiation of the measured data. A disadvantage of this approach is that minimization is usually nonlinear and often nonconvex. Various optimization algorithms have been used to perform the minimization. In general, an algorithm starts from a set of initial estimates of the parameters and improves it in an iterative manner until the system model response is sufficiently close to that of the observations.

Control-oriented techniques, stemming from the concept of quasilinearization of Bellman and Kalaba [1965], have been developed for aquifer parameter identification. Among the

TABLE 1. Parameter Identification Models, Equation Error Criteria

Applicable Conditions	Numerical Method	Parameters to be Identified	Data Processing	Prior Information or Constraints	Inverse Solution Procedure	Special Features and Comments	Reference
Two or three dimensional, confined/unconfined, steady state	finite difference	K, T	none	none			Nelson [1960, 1961]
Two or three dimensional, confined/unconfined, unsteady state		K, T	generalized orthogonal regression	boundary condition in permeability	energy dissipation method		Nelson [1968]
Two dimensional, confined unsteady state		T, S	none	none	linear programming		Kleinecke [1971]
Two dimensional, confined, steady-unsteady state		T, S, Q	none	flatness of parameters	minimizing norm of error flow matrix inverse	gradually increasing the number of zones $T(x, y)$ is represented by finite element	Emsellem and de Marsily [1971] Frind and Pinder [1973]
Two dimensional, confined, steady state,	finite element	T	none	T known along a line crossed by all streamlines			
Two dimensional, confined, steady state, anisotropic	finite element	T_x, T_y	none	lower upper bound on parameters	parametric linear programming algebraic approach	penalty term used to control instability	Neuman [1973]
Two dimensional, unsteady state, isotropic/anisotropic		T_x, T_y, S, Q	spline or Lagrange interpolation	none		inverse problems are reduced locally to algebraic equations of small dimensions	Sagar et. al. [1975]
Two dimensional, confined, unsteady state	finite difference	T, S, Q	none	none	linear programming or quadratic programming	compares five different optimization criteria	Hejlez et. al. [1975]
Two dimensional, confined, unsteady state	finite difference	T, S	none	limitation on local variability of T initial estimates	direct integration of P.D.E. minimizing a quadratic objective function with penalty function		Nutbrown [1975]
Two dimensional, confined, unsteady state	finite difference	T, S	none		generalized matrix inversion		Navarro [1977]
Two dimensional, confined, unsteady state	finite difference	T	kriging	none		instability is controlled by parameterization; determines optimum parameter dimensions	Yeh et. al. [1983]

Table presents typical models in chronological order. K , hydraulic conductivity; T , transmissivity; S , storage coefficient; Q , sink/source.

published works in parameter identification we may mention the following: quasilinearization [Yeh and Tauze, 1971; DiStefano and Rath, 1975]; minimax and linear programming [Yeh and Becker, 1973]; and maximum principle [Lin and Yeh, 1974], Yakowitz and Noren [1976]. Vermuri and Karplus [1969] formulated the inverse problem in terms of optimal control and solved it by a gradient procedure. Chen et al. [1974] and Chavent [1975] also treated the problem in an optimal control approach and solved it by both a steepest descent method and conjugate gradient method. Kalman filtering techniques have also been proposed in the literature for parameter identification [McLaughlin, 1975; Wilson et al., 1978]. Kitanidis and Vomvoris [1983] used the technique of maximum likelihood estimation and kriging.

Mathematical programming techniques developed in the field of operations research have been utilized for solving the inverse problem of parameter identification in groundwater hydrology and in the field of petroleum engineering. Among the published works we may mention the following: gradient search procedures [Jacquard and Jain, 1965; Thomas et al., 1972]; decomposition and multilevel optimization [Haimès et al., 1968]; linear programming [Coats et al., 1970; Slater and Durrer, 1971; Yeh, 1975a, b]; quadratic programming [Yeh, 1975a, b; Chang and Yeh, 1976]; the Gauss-Newton method [Jahns, 1966; McLaughlin, 1975]; the modified Gauss-Newton method [Yoon and Yeh, 1976; Yeh and Yoon, 1976; Cooley, 1977, 1982]; the Newton-Raphson method [Neuman and Yakowitz, 1979]; and conjugate gradient method [Neuman, 1980]. Some typical parameter identification models, using the output error criterion, are tabulated in Table 2.

PROBLEM STATEMENT

We will use a typical groundwater flow equation to illustrate some typical techniques that have been used to solve the inverse problem. Consider an unsteady flow in an inhomogeneous, isotropic, and confined aquifer for which the governing equation can be represented by

$$\frac{\partial}{\partial x} \left(T \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(T \frac{\partial h}{\partial y} \right) = Q + S \frac{\partial h}{\partial t} \quad (1)$$

subject to the following initial and boundary conditions:

$$\begin{aligned} h(x, y, 0) &= h_0(x, y) & x, y \in \Omega \\ h(x, y, t) &= h_1(x, y, t) & x, y, \in \partial\Omega_1 \\ T \frac{\partial h}{\partial n} &= h_2(x, y, t) & x, y \in \partial\Omega_2 \end{aligned} \quad (2)$$

where

$h(x, y, t)$	head;
$T(x, y)$	transmissivity;
S	storage coefficient;
$Q(x, y)$	source-sink term (known);
x, y	space variables;
t	time;
Ω	flow region;
$\partial\Omega$	boundary of the aquifer ($\partial\Omega_1 \cup \partial\Omega_2 = \partial\Omega$);
$\partial/\partial n$	normal derivative;
h_0, h_1, h_2	specified functions.

For illustrational purposes, let us assume that the storage coefficient is known and the parameter chosen for identification is the transmissivity function, $T(x, y)$, which is assumed to be time invariant. In general, a numerical scheme is required to obtain solutions of (1) subject to conditions (2), pro-

vided that parameter values are properly estimated. Various finite-difference or finite-element methods have been developed for numerical simulation studies. In solving the inverse problem, it is essential to have an efficient forward solution scheme, particularly when using an iterative nonlinear least square estimation. An example is the following classical Crank-Nicolson scheme:

$$\begin{aligned} & \frac{1}{2} [T_{i+1/2,j}(h_{i+1,j}^{n+1} - h_{i,j}^{n+1})/(\Delta x)^2 \\ & - T_{i-1/2,j}(h_{i,j}^{n+1} - h_{i-1,j}^{n+1})/(\Delta x)^2 \\ & + T_{i+1/2,j}(h_{i+1,j}^n - h_{i,j}^n)/(\Delta x)^2 \\ & - T_{i-1/2,j}(h_{i,j}^n - h_{i-1,j}^n)/(\Delta x)^2] \\ & + \frac{1}{2} [T_{i,j+1/2}(h_{i,j+1}^{n+1} - h_{i,j}^{n+1})/(\Delta y)^2 \\ & - T_{i,j-1/2}(h_{i,j}^{n+1} - h_{i,j-1}^{n+1})/(\Delta y)^2 \\ & + T_{i,j+1/2}(h_{i,j+1}^n - h_{i,j}^n) \\ & - T_{i,j-1/2}(h_{i,j}^n - h_{i,j-1}^n)/(\Delta y)^2] \\ & = Q_{i,j} + S(h_{i,j}^{n+1} - h_{i,j}^n)/\Delta t \end{aligned} \quad (3)$$

The above finite-difference equations can be solved by an alternating direction method [Douglas, 1962], which is locally second-order correct in space and time.

PARAMETER DIMENSION AND PARAMETERIZATION

Parameters, such as transmissivity, are continuous functions of the spatial variables. For identification purposes, a continuous function must be approximated by a finite dimensional form. The reduction of parameter dimension is done by parameterization. There are two ways that have been proposed in the literature.

Zonation Method

In this approach, the flow region is divided into a number of subregions, or zones, and a constant parameter value is used to characterize each zone. The unknown transmissivity function is then represented by a number of constants which is equal to the number of zones. Hence the dimension of parameterization (or parameter dimension) is then represented by the number of zones. Here, we mention the work of Coats et al. [1970], Emsellem and de Marsily [1971], Yeh and Yoon [1976], and Cooley [1977, 1979].

Interpolation Method

If finite elements are used as the interpolation method, the flow region is divided into a number of elements connected by a number of nodes. Each node is associated with a chosen local basis function. The unknown transmissivity function is then approximated by a linear combination of the basis functions, where the parameter dimension corresponds to the number of unknown nodal transmissivity values. Here, we mention the work of DiStefano and Rath [1975], Yoon and Yeh [1976], and Yeh and Yoon [1981]. In the context of interpolation, other schemes have also been used to approximate the transmissivity distribution, such as spline [Sagar et al., 1975; Yakowitz and Noren, 1976], polynomial method [Garay et al., 1976], and kriging [Clifton and Neuman, 1982]. The reduction of the number of unknown parameters by representing the parameters by a geostatistical structure as suggested by Kitanidis and Vomvoris [1983] can also be classified under the interpolation method.

However, one problem still remains, i.e., how to optimally determine the shape of zones in the zonation case or how to

optimally determine the location of nodes (nodal transmissivities) in the interpolation case. Most of the published work relies upon a trial-and-error approach or hydrological mapping. However, a recent paper by Sun and Yeh [1985] suggests a systematic way to identify the parameter structure.

INVERSE SOLUTION METHODS

Generalized Matrix Method Based Upon the Equation Error Criterion

When equation error criterion is employed for parameter estimation, it requires an explicit formulation of the unknown parameters. Suppose head observations are available at each of the grid points and these observations are substituted into (3); then the Crank-Nicolson scheme can be rewritten as

$$\begin{aligned} & (h_{i+1,j}^{n+1/2} - h_{i,j}^{n+1/2})T_{i+1,j} - (h_{i,j}^{n+1/2} \\ & - h_{i-1,j}^{n+1/2})T_{i-1,j} + (h_{i,j+1}^{n+1/2} - h_{i,j}^{n+1/2})T_{i,j+1} \\ & - (h_{i,j}^{n+1/2} - h_{i,j-1}^{n+1/2})T_{i,j-1} + (h_{i+1,j}^{n+1/2} \\ & + h_{i-1,j}^{n+1/2} + h_{i,j+1}^{n+1/2} + h_{i,j-1}^{n+1/2} - 4h_{i,j}^{n+1/2})T_{i,j} \\ & = \frac{2(\Delta x)^2}{\Delta t} S(h_{i,j}^{n+1} - h_{i,j}^n) + 2(\Delta x)^2 Q + \varepsilon_{i,j}^{n+1/2} \end{aligned} \quad (4)$$

where Δy is assumed to be equal to Δx , and

$$\begin{aligned} h_{i,j}^{n+1/2} &= \frac{1}{2}(h_{i,j}^n + h_{i,j}^{n+1}) \\ T_{i+1/2,j} &= \frac{1}{2}(T_{i,j} + T_{i+1,j}) \end{aligned}$$

To account for the lack of equality, an unknown error term $\varepsilon_{i,j}^{n+1/2}$ is added to (4). In practice, only a limited number of field observations is available. Interpolation schemes, such as cubic splines [Yakowitz and Noren, 1976] and kriging [Yeh et al., 1983] have been used in the past to obtain head values at every computational grid associated with the numerical scheme that is based upon either finite-difference or finite-element approximations. The error term consists of interpolation errors as well as noise in observations. Equation (4) can be simplified to

$$A_t T_g = b_t + \varepsilon_t \quad t = 1, 2, \dots, N \quad (5)$$

where

- A_t coefficient matrix, a function of h ;
- T_g transmissivity vector containing transmissivity values at all grid points;
- N total number of time steps;
- b_t column vector, a function of h .

In a more compact matrix form, this becomes

$$A T_g = b + \varepsilon \quad (6)$$

where

$$\begin{aligned} A &= [A_1^T, A_2^T, \dots, A_N^T]^T \\ b &= [b_1^T, b_2^T, \dots, b_N^T]^T \\ \varepsilon &= [\varepsilon_1^T, \varepsilon_2^T, \dots, \varepsilon_N^T]^T \end{aligned}$$

T is a transpose operator when used as a superscript. It should be noted that whether finite difference or finite element is used as the forward solution method, the resulting equation error will always have the form of (6). However, we have used a typical finite-difference method to demonstrate how to formulate the inverse problem by the equation error criterion. The advantage of this formulation is that (6) is linear, and T_g can be determined by minimizing the equation error ε .

From (6), the least squares error (or residual sum of squares)

can be expressed by

$$\varepsilon^T \varepsilon = (A T_g - b)^T (A T_g - b) \quad (7)$$

Minimizing the least square error, the transmissivity vector can be estimated as

$$\hat{T}_g = (A^T A)^{-1} A^T b \quad (8)$$

where \hat{T}_g is the estimated transmissivity vector of T_g . Note that solution (8) implicitly assumes homoscedasticity and lack of correlation among residuals. The solution is also highly dependent on the level of discretization used in the numerical solution of the governing equation. Another disadvantage is that solution of (8) is generally unstable in the presence of noise.

Gauss-Newton Minimization Based Upon the Output Error Criterion

For modeling purposes, the objective is to determine $T(x, y)$ from a limited number of observations of $h(x, y, t)$ scattered in the field so that a certain criterion is optimized. If the classical least square error is used to represent the output error, the objective function to be minimized is

$$\min_{T(x, y)} J = [h_D - h_D^*]^T [h_D - h_D^*] \quad (9)$$

where h_D is the vector of calculated heads at observation wells, based upon some estimated values of parameters, and h_D^* is the vector of observed heads.

For identification purposes, $T(x, y)$ can be parameterized by either a zonation or interpolation method as mentioned earlier.

The Gauss-Newton algorithm has proven to be an effective algorithm to perform minimization. The original and modified version of the algorithm has been used by many researchers in the past in solving the inverse problem, e.g., Jacquard and Jain [1965]; Jahns [1966], Thomas et al. [1972], Gavalas et al. [1976], Yoon and Yeh [1976], and Cooley [1977, 1982]. The popularity of the algorithm stems from the fact that it does not require the calculation of the Hessian matrix as is required by the Newton method and the rate of convergence is superior when compared to the classical gradient searching procedures. The algorithm is basically developed for unconstrained minimization. However, constraints such as upper and lower bounds are easily incorporated in the algorithm with minor modifications. The algorithm starts with a set of initial estimates of parameters and converges to a local optimum. If the objective function is convex, the local optimum would be the global optimum. Due to the presence of noise in the observations, the inverse problem is usually nonconvex, and hence only a local optimum can be assured in the minimization.

Let \bar{T} be a vector of parameters that contains $[T_1, T_2, \dots, T_L]$. The algorithm generates the following parameter sequence for an unconstrained minimization problem:

$$\bar{T}^{k+1} = \bar{T}^k - \rho^k d^k \quad (10)$$

with

$$A^k d^k = g^k \quad (11)$$

where

- $A^k = [J_D(\bar{T}^k)]^T [J_D(\bar{T}^k)]$, ($L \times L$);
- $g^k = [J_D(\bar{T}^k)]^T [h_D(\bar{T}^k) - h_D^*]$, ($L \times 1$);
- J_D Jacobian matrix of head with respect to \bar{T} , ($M \times L$);
- ρ^k step size, (scalar);
- d^k Gauss-Newton direction vector, ($L \times 1$);
- M number of observations;
- L parameter dimension.

TABLE 2. Parameter Identification Models, Output Error Criteria

Applicable Conditions	Numerical Method	Parameters to be Identified	Prior Information or Constraints	Inverse Solution Procedure	Special Features and Comments	Reference
Two dimensional, confined, unsteady state	finite difference	T, S	none	Gauss-Newton	for oil reservoir	<i>Jacquard and Jain</i> [1965]
Two dimensional, confined, unsteady state	finite difference	T, S	none	Gauss-Newton	statistical measures of estimated parameters are provided; for oil reservoir	<i>Jahns</i> [1966]
Two dimensional, unconfined unsteady state	finite difference	K, S	none	maximum principle in conjunction with steepest descent method	quazilinearization computation carried out on a hybrid computer	<i>Vemuri and Karplus</i> [1969]
One dimensional, unconfined, unsteady state	finite difference	D	none	quazilinearization		<i>Yeh and Tauxe</i> [1971]
Two dimensional, unsteady state	finite difference	K, ϕ	upper-lower bounds on parameters	Gauss-Newton, step size is determined by quadratic interpolation	box-type constraints are imposed on parameters; for oil reservoir	<i>Thomas et. al.</i> [1972]
One dimensional, leaky aquifer, unsteady state	finite difference	$T, S, K'/b'$	none	quazilinearization	radial flow	<i>Marino and Yeh</i> [1973]
Two dimensional, unsteady state	finite difference	K, ϕ	none	steepest descent and conjugate gradient	parameters are considered as continuous function of position; gradients obtained by optimal control theory	<i>Chen et. al.</i> [1974]
Two dimensional, unsteady state	finite difference	K, ϕ	upper-lower bounds on parameters	steepest descent	for oil reservoir; gradients are generated by solving the adjoint model	<i>Chavent et. al.</i> [1975]
One dimensional, unconfined, unsteady state	finite difference	D	none	quazilinearization; maximum principle; gradient; influence coefficient; linear programming	compares five different algorithms	<i>Yeh</i> [1975a]
One dimensional, confined, unsteady state	finite difference	D	upper and lower bounds; linear constraints	quadratic programming	radial flow	<i>Yeh</i> [1975b]
Two dimensional, confined, unsteady state	finite element	T	structure constraints	quazilinearization	transmissivity function is represented by finite element	<i>Distefano and Rath</i> [1975]
One dimensional	finite difference	K, ϕ	mean and covariance matrix of parameters	conjugate gradient, Gauss-Newton, Marquardt	a Bayesian penalty term is added to the objective function	<i>Gavalas et. al.</i> [1976]
Two dimensional confined, unsteady state	finite element	K	upper-lower bounds on parameters	Gauss-Newton with Rosen's gradient projection	permeability function is represented by finite element	<i>Yoon and Yeh</i> [1976]
Two dimensional unconfined, unsteady state	finite difference	T	upper-lower bounds on parameters	Gauss-Newton with Rosen's gradient projection	stepwise zoning procedure using statistical measures of parameters; covariance matrix of estimated parameters is provided	<i>Yeh and Yoon</i> [1976]
Two dimensional, steady state	finite element	K, Q flux	none	modified Gauss-Newton (nonlinear regression by linearization)	statistical measures of model and parameters are provided	<i>Cooley</i> [1977]
One dimensional		ϕ, k	mean and covariance matrix of parameters	Gauss-Newton	for oil reservoir; covariance matrix of estimated parameter is provided; determines optimum level of parameterization	<i>Shah et. al.</i> [1978]
Two dimensional steady state	finite element	T	prior estimation of parameters added to objective	Newton-Raphson	covariance matrix of parameter estimates is provided	<i>Neuman and Yakowitz</i> [1979]

TABLE 2. (continued)

Applicable Conditions	Numerical Method	Parameters to be Identified	Prior Information or Constraints	Inverse Solution Procedure	Special Features and Comments	Reference
Two dimensional steady state	finite element	T	prior estimation of parameters added to objective	Conjugate gradient	variational theory is used; use log transmissivities	Neuman [1980]
Two dimensional confined, unsteady state	finite difference	T	upper-lower bounds on parameters	Gauss-Newton with Rosen's gradient projection	finite element is used to represent $T(x, y)$; determines optimum parameter dimension; considers parameter uncertainty	Yeh and Yoon [1981]
Two dimensional steady state	finite element	K, Q flux	prior estimates of parameters with or without reliability added to objective	modified Gauss-Newton (nonlinear regression by linearization)	two types of prior information are included in the analysis	Cooley [1982]
Steady state		K	point measurement of permeability and hydraulic head	maximum likelihood and kriging	parameter is represented as a "random field"	Kitanidis and Vomvoris [1983]
Two dimensional confined, unsteady state	finite element	K	none	Gauss-Newton with Rosen's gradient projection	generalized least squares; considers correlated errors	Sadeghipour and Yeh [1984]
Two dimensional steady state	finite difference	T	point measurements of transmissivity and head	cokriging	parameter is represented as a random field	Hoeksema and Kitanidis [1984]
Two dimensional confined, unsteady state	finite element	T	none	Gauss-Newton	identification of parameter structure	Sun and Yeh [1985]
Two dimensional, steady state	analytical solution	T	point measurements of transmissivity and head	Gaussian conditioned mean	parameter is represented as a random field	Dagan [1985]
Two dimensional steady state, leakage included	finite difference	T	point measurements of transmissivity and head		comparison of Gaussian conditional mean and kriging estimation	Hoeksema and Kitanidis [1985]

Table presents typical models in chronological order. D , diffusivity; ϕ , porosity. See Table 1 for additional definitions.

The step size ρ^k , a scalar, can be determined by a quadratic interpolation scheme such that $J(\bar{T}^{k+1}) < J(\bar{T}^k)$, or simply by a trial-and-error procedure. Occasionally, the direction matrix $[J_D^T J_D]$ may become ill-conditioned. Corrections must be made in order for the algorithm to continue, and the methods suggested by Levenberg [1944] and Marquardt [1963] are a modification of the Gauss-Newton direction. As stated earlier, the basic Gauss-Newton algorithm does not handle constraints. If constraints are imposed on the parameters, such as the upper and lower bounds, the Gauss-Newton algorithm can be allied with a gradient projection technique.

The elements of the Jacobian matrix are represented by the sensitivity coefficients,

$$J_D = \begin{bmatrix} \frac{\partial h_1}{\partial T_1} & \frac{\partial h_1}{\partial T_2} & \dots & \frac{\partial h_1}{\partial T_L} \\ \frac{\partial h_2}{\partial T_1} & \frac{\partial h_2}{\partial T_2} & \dots & \frac{\partial h_2}{\partial T_L} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial h_M}{\partial T_1} & \frac{\partial h_M}{\partial T_2} & \dots & \frac{\partial h_M}{\partial T_L} \end{bmatrix} \quad (12)$$

where M is the total number of observations, and L is the total number of parameters. The transpose of the Jacobian

matrix is

$$J_D^T = \begin{bmatrix} \frac{\partial h_1}{\partial T_1} & \frac{\partial h_2}{\partial T_1} & \dots & \frac{\partial h_M}{\partial T_1} \\ \frac{\partial h_1}{\partial T_2} & \frac{\partial h_2}{\partial T_2} & \dots & \frac{\partial h_M}{\partial T_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial h_1}{\partial T_L} & \frac{\partial h_2}{\partial T_L} & \dots & \frac{\partial h_M}{\partial T_L} \end{bmatrix} \quad (13)$$

In solving the inverse problem, an efficient method must be used in the calculation of the sensitivity coefficients. We will now focus our attention on the techniques developed for calculating the sensitivity coefficients.

COMPUTATION OF SENSITIVITY COEFFICIENTS

Sensitivity coefficients, the partial derivatives of head with respect to each of the parameters, play an important role in the solution of the inverse problem. In the Gauss-Newton algorithm, elements of the Jacobian matrix are represented by the sensitivity coefficients, $\partial h_i / \partial T_l$, $i = 1, \dots, M$, $l = 1, \dots, L$. If h is the head vector, the sensitivity coefficients are $\partial h / \partial T_l$, $l = 1, \dots, L$. Literature review indicates that three methods

have been used in the past in the calculation of sensitivity coefficients. We will summarize these methods as follows.

Influence Coefficient Method

The Influence Coefficient method [Becker and Yeh, 1972] uses the concept of parameter perturbation. The *l*th row of J_D^T is approximated by

$$\frac{\partial h_i}{\partial T_l} \approx \frac{h_i(\bar{T} + \Delta T_l e_l) - h_i(\bar{T})}{\Delta T_l} \quad i = 1, \dots, M \quad (14)$$

where ΔT_l is the small increment of T_l , and e_l is the *l*th unit vector. The values of $h(\bar{T})$ and $h(\bar{T} + \Delta T_l e_l)$ are obtained by solving the governing equation (by simulation), subject to the imposed initial and boundary conditions. The method requires perturbing each parameter one at a time. If there are *L* parameters to be identified, the governing equation has to be solved (simulated) (*L* + 1) times for each iteration in the nonlinear least squares minimization to numerically produce the sensitivity coefficients. The numerical representation of J_D^T is called the influence coefficient matrix [Becker and Yeh, 1972]. The elements of the influence coefficient matrix, represented by a_{i1} , are numerical approximations of the sensitivity coefficients,

$$\begin{matrix} & h_1 & h_2 & \dots & h_M \\ T_1 & a_{11} & a_{12} & \dots & a_{1M} \\ T_2 & a_{21} & a_{22} & \dots & a_{2M} \\ \dots & \dots & \dots & \dots & \dots \\ T_L & a_{L1} & a_{L2} & \dots & a_{LM} \end{matrix} \quad (15)$$

Each element in the matrix represents the ratio of change in the head to the change in a particular parameter. The value of ΔT_l is a small increment of T_l by which parameter T_l is perturbed. The appropriate value of ΔT_l is usually determined on a trial-and-error basis. Bard [1974] has suggested some guidelines in choosing the value of ΔT_l .

Sensitivity Equation Method

In this approach, a set of sensitivity equations are obtained by taking the partial derivatives with respect to each parameter in the governing equation and initial and boundary conditions. After taking the partial derivatives, the following set of sensitivity equations result:

$$\begin{aligned} \frac{\partial}{\partial x} \left[T \frac{\partial \left(\frac{\partial h}{\partial T_l} \right)}{\partial x} \right] + \frac{\partial}{\partial y} \left[T \frac{\partial \left(\frac{\partial h}{\partial T_l} \right)}{\partial y} \right] &= S \frac{\partial \left(\frac{\partial h}{\partial T_l} \right)}{\partial t} \\ + \left[-\frac{\partial}{\partial x} \left(\frac{\partial T}{\partial T_l} \frac{\partial h}{\partial x} \right) - \frac{\partial}{\partial y} \left(\frac{\partial T}{\partial T_l} \frac{\partial h}{\partial y} \right) \right] & \quad l = 1, \dots, L \end{aligned} \quad (16)$$

The associated initial and boundary condition are

$$\begin{aligned} \frac{\partial h(x, y, 0)}{\partial T_l} &= 0 \quad l = 1, \dots, L \\ \frac{\partial h(x, y, t)}{\partial T_l} &= 0 \quad l = 1, \dots, L \\ T \frac{\partial \left(\frac{\partial h}{\partial T_l} \right)}{\partial n} &= -\frac{\partial T}{\partial T_l} \frac{\partial h}{\partial n} \quad l = 1, \dots, L \end{aligned} \quad (17)$$

The numerical values of $\partial h/\partial x$ and $\partial h/\partial y$ are obtained from the solution of the governing equation. If we replace $(\partial h/\partial T_l)$

by *h* and consider the term

$$\left[-\frac{\partial}{\partial x} \left(\frac{\partial T}{\partial T_l} \frac{\partial h}{\partial x} \right) - \frac{\partial}{\partial y} \left(\frac{\partial T}{\partial T_l} \frac{\partial h}{\partial y} \right) \right]$$

as *Q*, the set of sensitivity equations would be of the same form as that of the governing equation. Hence the solution method used for solving the governing equation can be used to solve the set of sensitivity equations. The number of simulation runs required to generate the sensitivity coefficients per iteration is (*L* + 1), which is the same as that of the influence coefficient method.

Variational Method

The variational method was first used for solving the inverse problem of parameter identification by Jacquard and Jain [1965] and then by Carter et al. [1974, 1982] associated with finite difference schemes. Sun and Yeh [1985] extended the method to the case of a finite element scheme. Following Carter et al., [1974], the sensitivity coefficients can be computed by the following equation:

$$\frac{\partial h^{(j)}}{\partial T_l^{(i)}} = \iint_{(\Omega_i)} \int_0^t \nabla q'(x, y, t - \tau) \nabla h(x, y, \tau) d\tau dx dy \quad (18)$$

$j = 1, 2, \dots, N_0 \quad i = 1, 2, \dots, N_n$

where (Ω_i) is the exclusive subdomain of node *i* as defined by Sun and Yeh; ∇ is the gradient operator; $h(x, y, t)$ is the solution of the governing equation; N_0 is the number of observation wells; N_n is the total number of nodes used in the numerical solution; $q'(x, y, t)$ is the time derivative of $q(x, y, t)$, which is the solution of the following set of adjoint equations:

$$\frac{\partial}{\partial x} \left[T \frac{\partial q}{\partial x} \right] + \frac{\partial}{\partial y} \left[T \frac{\partial q}{\partial y} \right] = S \frac{\partial q}{\partial t} + G_j(x, y)H(t) \quad (19)$$

subject to the following initial and boundary conditions:

$$\begin{aligned} q(x, y, 0) &= 0 \quad (x, y) \in \Omega \\ q(x, y, t) &= 0 \quad (x, y) \in \partial\Omega_1 \\ \frac{\partial q}{\partial n}(x, y, t) &= 0 \quad (x, y) \in \partial\Omega_2 \end{aligned} \quad (20)$$

where

$$\begin{aligned} G_j(x, y) &= \frac{1}{P_j} \quad (x, y) \in (\Omega_j) \\ G_j(x, y) &= 0 \quad \text{otherwise} \\ H(t) &= 0 \quad t \leq 0 \\ H(t) &= 1 \quad t > 0 \end{aligned} \quad (21)$$

P_j is the area of subdomain (Ω_j) .

Note that the adjoint equation for $q(x, y, t)$ (equation (19)) has the same form as that of the governing equation for $h(x, y, t)$ (equation (1)), and hence the same numerical scheme can be used to solve *h* and *q*. By solving the governing equation one time only and solving the adjoint equation for each observation well, all sensitivity coefficients, $[(\partial h^{(j)})/\partial T_l^{(i)}]$ ($j = 1, 2, \dots, N_0; i = 1, 2, \dots, N_n$), can be produced. Hence the number of simulation runs required to calculate the sensitivity coefficients per iteration is ($N_0 + 1$), as compared to (*L* + 1), which is required by either the influence coefficient method or the sensitivity equation method.

Comparing the above-mentioned three methods in the cal-

ulation of sensitivity coefficients, it is clear that the variational method would be advantageous if $L > N_0$, the case where the number of parameters to be identified is greater than the number of observation wells. On the other hand, if $N_0 > L$, the influence coefficient and sensitivity equation methods are preferred. To avoid instability when data contains noise, the number of parameters to be identified is usually less than the number of observation wells. In using the sensitivity equation method, caution must be exercised in that $\partial h_i / \partial T_i$ varies much more rapidly with time than h . DiStefano and Rath [1975] pointed out that in order to obtain a set of sensitivity coefficients with acceptable accuracy, much smaller time steps are required in the simulation runs. Whereas in the influence coefficient method, the perturbation vector $\Delta \bar{T}$ can be appropriately chosen to cause sufficient change in $h(\bar{T}, t)$ and yet small enough so that numerical approximations of sensitivity coefficients are valid. However, the sensitivity and variational methods are intrinsically much more accurate. The need for an efficient method for calculating the sensitivity coefficients in solving inverse problems has also been pointed out by Dogru and Seinfeld [1981], McElwee [1982], and Sykes et al. [1985].

PARAMETER UNCERTAINTY AND OPTIMUM PARAMETER DIMENSION

The identification of parameters in a distributed parameter system should, in principle, include the determination of both the parameter structure and its value. If zonation is used to parameterize the unknown parameters, parameter structure is represented by the number and shape of zones. On the other hand, if finite element is used for parameterization, parameter structure concerns the number and location of nodal values of parameters. Emsellem and de Marsily [1971] were the first to consider the problem of optimal zoning pattern. Yeh and Yoon [1976] suggested a systematic procedure based upon a statistical criterion for the determination of an optimum zoning pattern. Shah et al. [1978] showed the relationship between the optimal dimension of parameterization and observations in considerable depth. The necessity to limit the dimension of parameterization has been further studied by Yeh and Yoon [1981] and Yeh et al. [1983] and Kitanidis and Vomvoris [1983]. The dimension of parameterization is directly related to the quantity and quality of data (observations). In field practice, the number of observations is limited and observations are corrupted with noise. Without controlling parameter dimension, instability often results [Yakowitz and Duckstein, 1980]. If instability occurs in the inverse problem solution, parameters will become unreasonably small (sometimes negative, which is physically impossible) and/or large, if parameters are not constrained. In the constrained minimization, instability is characterized by the fact that during the solution process parameter values are bouncing back and forth between the upper and lower bounds. Reduction of parameter dimension can make the inverse solution stable. It has been generally understood that as the number of zones (in the zonation case) is increased, the modeling error (least squares) decreases while the error in parameter uncertainty increases. A trade off of the two types of errors can then be made from which an optimum parameter dimension can be determined. A standard procedure is to gradually increase the parameter dimension, starting from the homogeneous case, and calculate the two types of errors for each parameter dimension. The error in parameter uncertainty can be represented by a norm of the covariance matrix of the estimated parameters [Yeh and Yoon, 1976; Shah et al., 1978].

Calculation of Statistics

The covariance matrix of the estimated parameters is defined by

$$\text{Cov}(\hat{T}) = E\{(\bar{T} - \hat{T})(\bar{T} - \hat{T})^T\} \quad (22)$$

where

- \hat{T} estimated parameters;
- \bar{T} true parameters;
- E mathematical expectation;
- T transpose of a vector when used as superscript.

An approximation of the covariance matrix of the estimated parameters in nonlinear regression can be represented by the following form [Bard, 1974; Yeh and Yoon, 1976, 1981; Shah et al., 1978]:

$$\text{Cov}(\hat{T}) = \frac{J(\hat{T})}{M - L} [A(T)]^{-1} \quad (23)$$

where

- $J(\hat{T})$ least squares error;
- M number of observations;
- L parameter dimension;
- A $[J_D^T J_D]$;
- J_D Jacobian matrix of h with respect to T .

A norm of the covariance matrix has been used to represent the error in parameter uncertainty. Norms, such as trace, spectral radius (maximum eigen value), and determinant have been used in the literature. Equation (23) also assumes homoscedasticity and uncorrelated errors. This assumption is generally not satisfied and the actual covariance may be much higher than that given by (23).

The covariance matrix of the estimated parameters also provides information regarding the reliability of each of the estimated parameters. A well-estimated parameter is generally characterized by a small variance as compared to an insensitive parameter that is associated with a large variance. By definition, the correlation matrix of the estimated parameters is

$$\bar{R} = \begin{bmatrix} \frac{c_{11}}{(c_{11}c_{11})^{1/2}} & \cdots & \frac{c_{1L}}{(c_{11}c_{LL})^{1/2}} \\ \frac{c_{L1}}{(c_{LL}c_{11})^{1/2}} & \cdots & \frac{c_{LL}}{(c_{LL}c_{LL})^{1/2}} \end{bmatrix} \quad (24)$$

where c_{ij} 's are elements of the covariance matrix of the estimated parameter. The more sensitive the parameter, the closer and quicker the parameter will converge. A correlation analysis of the estimated parameters would indicate the degree of interdependence among the parameters with respect to the objective function. Correlation of parameters is called the collinearity problem. Such problem can cause slow rate of convergence in minimization and in most cases result in nonoptimal parameter estimates. A more rigorous treatment of the collinearity problem is to use the more sophisticated statistical techniques, such as ridge regression [Cooley, 1977] and the method of principal components.

Cooley [1977] treated the inverse problem as a problem in nonlinear regression. A finite element scheme was used to solve the confined, steady state groundwater flow equation. The parameters identified included transmissivity, hydraulic conductance, source-sink strength, and boundary flux. The nonlinear system of normal equations was solved by the technique of quasilinearization [Bellman and Kalaba, 1965] and a modified Gauss-Newton algorithm. Beale's nonlinearity mea-

sure was used to test the applicability of linear statistical analysis for the original nonlinear regression problem. The advantage of using a standard regression procedure for parameter identification is that it allows for the application of established, formal statistical techniques for testing the validity of assumptions and model fit as well as estimating the reliability and significance of the model and its parameters. However, caution must be exercised, since statistics derived from linear statistical theory are not strictly applicable to the nonlinear case.

BAYESIAN ESTIMATION

Bayesian estimation methods that incorporate prior information have also been applied to parameter identification [e.g., Gavalas *et al.*, 1976]. The geological information required for Bayesian estimation includes the mean and covariance matrix of the parameters which are

$$E\{\bar{T}\} = T_{\text{mean}} \quad (25)$$

$$E\{(T_i - T_{\text{mean}})(T_j - T_{\text{mean}})\} = r_{ij} \quad (26)$$

The values of T_{mean} and $R(r_{ij})$ are considered to be known and are the prior information which can be obtained from geological measurements in the field. Gavalas *et al.* have shown that Bayesian estimation reduces to a quadratic minimization problem, provided the parameters and the measurement errors are normally distributed and the model is linear in the parameters. When these conditions are not satisfied, a rigorous application of Bayesian estimation is impractical.

Composite Objective Function

Gavalas *et al.* [1976] proposed the following practical approach which is akin to least squares minimization where the objective function is

$$J = \sum_{i=1}^M \frac{1}{\sigma_i^2} (h_i - h_i^*)^2 + \lambda (\bar{T} - T_{\text{mean}})^T R^{-1} (\bar{T} - T_{\text{mean}}) \quad (27)$$

where λ is a weighting factor ($0 \leq \lambda \leq 1$) and σ_i^2 , $i = 1, 2, \dots$, M is the variance of the measurement error which is considered to be known. The second term in the objective function is the Bayesian term which penalizes the weighted deviation of the parameters from their mean value. It, in turn, requires the parameter to follow some preconceived pattern during the minimization process. Shah *et al.* [1978] have demonstrated that if reliable prior information is available, Bayesian estimation will lead to a smaller variance of the error of estimation.

Kalman Filter

The technique of Kalman filtering was originally developed in the field of optimal control [Kalman, 1960]. It has been successfully applied in aerospace engineering for the problem of optimal estimation and control of vehicle trajectory. The application of Kalman filtering to parameter estimation in groundwater requires expressing the groundwater model in terms of a state-space formulation that consists of a vector state equation and a vector observation equation. For parameter estimation, the state vector is augmented to include the parameter vector as another state variable. If the errors in the state and observation equations have zero mean and are of white Gaussian process with known covariance matrices, Kalman filtering can be applied for simultaneous, recursive state, and parameter estimation. Since prior information is generally required in the application of Kalman filtering, it can be classified in the Bayesian estimation category. Wilson

et al. [1978] used an extended Kalman filter for parameter estimation in groundwater. Their approach permits the utilization of prior information about the parameters and information taken from input-output measurements to improve estimates of parameters as well as the system state.

OTHER STATISTICAL METHODS THAT INCORPORATE PRIOR INFORMATION

Neuman and Yakowitz [1979] proposed a statistical approach to the inverse problem of parameter estimation. Their approach differs from the Bayesian estimation of Gavalas *et al.* [1976] in that the prior information may include actual values of transmissivity determined from pumping tests or other measurements at specific locations in the aquifer, or it may be based on statistical information about the spatial variability of transmissivities (not their actual values) in other aquifers consisting of similar materials [Neuman and Yakowitz, 1979]. The composite least squares criterion proposed by Neuman and Yakowitz is similar to (27) and can be expressed as

$$J = [h^* - f(\bar{T})]^T V_h^{-1} [h^* - f(\bar{T})] + \lambda (T^* - \bar{T})^T V_T^{-1} (T^* - \bar{T}) \quad (28)$$

where

- T^* prior estimate of \bar{T} ;
- V_T known symmetric positive definite matrix;
- V_h known matrix, symmetric and positive definite;
- λ unknown positive parameter;
- $f(\bar{T})$ model solution;
- h^* observed head.

The observed head (h^*) and the prior estimates of transmissivity (T^*) are related to true head (h) and true transmissivity (\bar{T}) by

$$\begin{aligned} h^* &= h + \varepsilon \\ T^* &= \bar{T} + v \end{aligned} \quad (29)$$

and

$$E(\varepsilon) = 0 \quad (30)$$

$$\text{Var}(\varepsilon) = \sigma_h^2 V_h$$

$$E(v) = 0 \quad (31)$$

$$\text{Var}(v) = \sigma_T^2 V_T$$

It is assumed that V_h and V_T are known, but σ_h and σ_T do not enter the computations. The second term in the composite objective function provides a smoothing effect in the minimization. Neuman and Yakowitz proposed two methods, called cross-validation and comparative residual analysis, to select the optimum value of λ . Neuman [1980] developed an efficient conjugate gradient algorithm for performing the minimization. He extended the variational method developed by Chavent [1975] for calculating the gradient with respect to the parameter in the case of generalized nonlinear least squares. The variational method presented by Chavent and Neuman is conceptually similar to Carter *et al.* [1974], but differs in the objectives. Carter *et al.* developed expressions which can be used to calculate the partial derivative of head with respect to the parameter, while Chavent and Neuman seek to compute the partial derivative of the least square criterion with respect to the parameter.

The composite objective function presented by Aboufirassi and Marino [1984b] is again conceptually similar to (27). They

used kriging to estimate the missing values of head and the value of the error covariance matrix, while cokriging [Abouf-rassi and Marino, 1984a] was used to estimate T^* and the associated error covariance matrix. Cokriging [Journal and Huijbregts, 1978], an extension of kriging to two or more variables, can be used to improve the accuracy of estimation of a variable that is not sufficiently sampled by considering its spatial correlation with other variables that are better sampled.

Cooley [1982] proposed a method to incorporate prior information on the parameters into the nonlinear regression model he developed [Cooley, 1977]. The primary purpose of Cooley's work is the incorporation of prior information of unknown reliability, the approach is an extension of ridge regression. A secondary objective of Cooley's work is to incorporate Theil's [1963] into Cooley's [1977] nonlinear regression model where at least some prior information of known reliability is available. The approach is non-Bayesian in the sense that no prior distribution of parameter is assumed. The approach also differs from the method proposed by Neuman and Yakowitz [1979] and Neuman [1980] primarily in two ways: (1) the prior information in Cooley's work is considered to consist of general nonlinear combinations of several types of parameters as opposed to direct estimates of a single type of parameter (transmissivity) and (2) the way in which the covariance structure of the model is determined. Nonstochastic prior information, as represented by a set of approximate linearized equations, is incorporated in the ridge regression previously developed by Cooley.

As was presented in Cooley [1982], the prior information having unknown reliability can be incorporated into the standard weighted least squares objective function by adding a penalty function. The resulting composite objective function consists of two terms. The first term is the weighted sum of squared errors in the hydraulic head, and the second term is sum of the weighted errors in the parameters. Cooley also introduced two scalars k and f in the composite objective function which can be adjusted to minimize the sum of the squared errors in the computed parameters.

Kitanidis and Vomvoris [1983] proposed a geostatistical approach for solving the inverse problem. Their method consists of two main steps: (1) the structure of the parameter field is identified, i.e., mathematical representations of the variogram and the trend are selected and their parameters are established, and (2) kriging is applied to provide minimum variance and unbiased point estimates of hydrogeological parameters using all available information. In their approach, it is assumed that several point measurements of head and transmissivities (in logarithms) are available. In effect, parameterization is achieved by representing the hydrogeological parameters as a random field which can be characterized by the variogram and trend with a small number of parameters. In fact, the parameters to be estimated at the first step are the ones associated with the variogram and trend, thus drastically reducing the parameter dimension. As was demonstrated by Kitanidis and Vomvoris [1983], the reduction of parameter dimension has resulted in stable inverse problem solutions with the presence of errors. Hoeksema and Kitanidis [1984] have applied the geostatistical approach to the case of two-dimensional steady state flow. A finite difference numerical model of groundwater flow was used to relate the head and transmissivity variability and cokriging was used to estimate the unknown transmissivity field. Dagan [1985] has also considered the geostatistical approach, but an analytical tech-

nique and Gaussian conditional mean are used in place of Kriging. Hoeksema and Kitanidis [1985] made a comparative study of Dagan's approach and Kriging estimation. In using the geostatistical approach, it is implicitly assumed that transmissivity has a low variability.

Correlation of error residuals, in both time and spatial domain, may occur for a number of reasons. Successive errors in time series tend to be positively correlated. Also, observations taken from adjacent pumping wells are affected by similar external conditions and may result in similar residuals. The presence of correlation in error terms suggests that there is additional information in the data that has to be included in the least squares minimization model. A well-established method which can be used to perform such minimization is the generalized least squares developed in the field of econometrics. In the case of an unsteady state flow, the error vector for each time period can be approximated by a stationary first-order autoregression process [Judge et al. 1980]. A method suggested by Sadeghipour and Yeh [1984] requires the estimation of lag-one serial coefficient (ρ) and the common covariance matrix (W) for the error vector. Using the estimated values of ρ and W , the generalized least squares method as demonstrated by Sadeghipour and Yeh provides parameter estimates with minimum variance when errors are correlated. If ρ and W are fixed and errors are normally distributed, the generalized least squares criterion corresponds to the log likelihood function.

In practice, ρ and W are unknown. Sadeghipour and Yeh [1984] proposed a two-step procedure. In step one, while assuming $\rho = 0$ and $W = I$, the minimization produces the ordinary least squares parameter estimates. These estimates are used to estimate ρ and W . In step two, the newly estimated ρ and W are used to perform the generalized least squares minimization. The process continues until convergence is reached.

SUMMARY AND FUTURE RESEARCH DIRECTION

The inverse problem of parameter identification has been classified by the performance criterion used in the solution. All published methods for solving the inverse problem belong to either the equation error approach or the output error approach. The output error criterion appears to be widely used not only in groundwater but also in oil reservoir problems. Optimization methods originally developed in the fields of optimal control and operations research have been adopted to perform minimization. Linear statistical methods have been used to establish the reliability of the estimated parameters. Bayesian type of approach has also been used to incorporate prior information. The inverse problem is inherently ill-posed. It has been made clear that parameterization is essential, i.e., the number of parameters to be identified must be limited. The number of parameters (parameter dimension) that can be identified for a given situation depends on the quantity and quality of the data. Identifiability must be relaxed, since measurements cannot be made at every spatial point as a function of time.

Suggested areas for future research are summarized as follows.

1. So far, only linear statistical methods have been used for testing the validity and assumptions and model fit as well as estimating the reliability and significance of the model and its parameters. However, the inverse problem in groundwater is basically nonlinear. Future research should be directed toward the development of nonlinear parameter estimation theories. However, caution must be exercised in that nonlinear methods are usually associated with high computational cost,

and their practical applicability must be examined in view of the fact that linear estimation methods have served well in many instances.

2. The primary purpose of incorporating the prior information into the inverse problem is to reduce the parameter uncertainty, not to improve the model fit. As a matter of fact, prior information can only worsen the model fit. The incorporation of prior information as a penalty function in the composite, least square objective function does not affect the feasible region of minimization. However, if prior information is used correctly the inverse solution will produce stable and reliable parameter estimates which will be more useful in groundwater management and prediction. It is also intuitively obvious that inaccurate prior information will degrade the parameter estimates. A future area of research is the development of reliable prior parameter estimates that are compatible with sample information.

3. It has been made clear that parameterization must include the parameter structure and its values. The development of an efficient and systematic parameter structure identification procedure continues to be a future area of research.

4. Due to its level of difficulty, the problem of identifiability has received little attention. However, some recently published results indicate that an extended identifiability can be used for groundwater modeling and management. A future area of research is to continue to study the problem of optimal pumping design in connection with aquifer parameter identification.

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