AQUIFER PARAMETER ESTIMATION BY QUASILINEARIZATION AND INVARIANT IMBEDDING

by

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CHAPTER 1

FUNDAMENTAL CONCEPTS

1.1 INTRODUCTION

A large class of simulation and mathematical models are often used in analyzing problems in engineering, science and industries. Most models are of parametric type in which parameters used in deriving the governing equation are not directly measurable and have to be determined from historical records. Frequently, they involve differential equations of two-point or multipoint boundary value type. In these problems, the boundary conditions are specified at two points or multi-points. To complicate the matter, the governing differential equations for a majority of such problems are nonlinear and cannot be solved analytically. The solutions must be obtained by numerical methods. Numerically, the difficulties are caused by the fact that not all the conditions are given at one point.

Methods for the numerical solution of such problems can be separated into two groups, the iterative and the non-iterative methods. Among such methods, quasilinearization and invariant imbedding, classified into the iterative and the non-iterative method, respectively, are presented. Quasilinearization is an iterative approach allied with linear approximation while invariant imbedding represents a completely different formulation of the original problem.

The purpose of this study is to use these two methods for estimating unknown parameters by obtaining numerical solutions of the problem of boundary value type in the groundwater aquifer and stream interaction system. Emphasis is therefore placed on the computational instead of the mathematical aspects of the methods. Most discussions are concerned with the computational requirements and the actual convergence rates. No detailed discussions concerning the groundwater aquifer and stream interaction system are given. Computational procedures are discussed in detail together with the numerical results.

The purpose of this chapter is to introduce the basic concepts used throughout the study. The parameter estimation problem is defined and explained briefly. The general concepts of quasilinearization and invariant imbedding are also introduced. More detailed explanations and applications about quasilinearization and invariant imbedding appear in later chapters.

Chapter 2 is devoted to the description and the analytical formulation of a problem concerning the groundwater aquifer and stream interaction system. Previous studies about the aquifer parameter estimation are reviewed. Hydrological background and simple definitions are also explained briefly.

The quasilinearization technique is detailed in Chapter 3 and applied to the parameter estimation problem in the groundwater aquifer system.

In Chapter 4, the estimation problem is treated by the concept of invariant imbedding. The nonlinear filtering theory is also discussed briefly.

An ITEL AS/5 computer was used throughout this work.

1.2 PARAMETER ESTIMATION

The parameter estimation problem, which is frequently called an inverse problem or a history matching problem, is a combination of experimental work with the mathematical aspects. In other words, it is the determination from experimental data of a set of unknown parameters in a mathematical model of a physical system, such that over a desired range of operating conditions the model outputs are close to the system outputs when the two are subject to analogous inputs. Parameters are defined as functions or constants, other than the dependent variables, which appear explicitly in the mathematical model. A distributed system, encountered frequently in groundwater systems, is defined as a system where the variables of importance are related by transformations or mappings which depend on local spatial variations as well as time.

In order to implement effective system control strategies, accurate system models are required. Usually, the parameters or coefficients used in deriving the governing equation cannot be measured directly; the measurable variables are the dependent variables of the differential equations. Thus, it is easily shown that to identify these parameters is not a simple matter. Much of classical and modern science and engineering has been concerned with this fundamental problem. Laboratory and experimental determination of chemical reaction rate constants, heat transfer coefficients, gas properties, diffusion constants, elastic moduli, transmissivities, etc. is an ongoing effort throughout the scientific world.

The steps involved in the parameter estimation can be the following (26):

1) Write the mathematical description, containing unknown parameters, of the system under consideration.
2) Choose a method to solve the mathematical description of the system.
3) Decide on measurement location(s) in the spatial domain.
4) Choose a criterion of performance.
5) Perform a sensitivity analysis.
6) Choose an optimization scheme.
7) Perform an error analysis.

By considering the step by step procedures involved in solving the parameter estimation problem, it is shown that such problems may be converted into standard optimization problems where any one of a number of optimization techniques may be used. In this way, not only the known structural configuration of the model but also the approximated values of the parameters are utilized.

1.3 QUASILINEARIZATION

The quasilinearization technique, which is often referred to as a generalized Newton-Raphson method for functional equations, involves decoupling the nonlinear differential equation by linearization into a series of linear differential equations that may be iteratively solved in such a way that their solutions converge to the solutions of the original problem. Thus, this algorithm is an iterative and indirect computational approach which usually requires a good initial approximation in order to converge. The main advantage of this technique is that it converges quadratically to the solution of the original problem if it converges at all.

The linearized equation is obtained simply by a Taylor's series expansion of the original nonlinear equation; only the linear terms are maintained.

Since linear differential equations of the boundary value type with variable coefficients can be solved easily on modern high speed computers by the principle of superposition (in this work, the method of complementary function), an efficient recursive formula has been developed (38).

1.4 INVARIANT IMBEDDING

Invariant imbedding is only a concept, which enables the transformation of boundary value problems into initial value problems by introducing new state variables and imbedding the original problem in a new family of similar problems. Although the actual application of the imbedding is relatively straightforward, the exact form of the imbedding to be used normally must be determined for each new problem.

In its basic concept, the approach involves generating a family of problems by means of a single parameter, where the basic properties of the system remain invariant. The new family then provides a means of advancing from one member to the solution of the original problem.

This concept can be applied to the various fields of science and engineering. Many problems of classical anaysis can also be viewed as an imbedding, where the imbedding is almost always either position in a fixed interval or time. Frequently, invariant imbedding gives new insights to the same problems treated by the classical anaysis because of its completely different approach.

CHAPTER 2

PROBLEM DESCRIPTION AND ANALYTICAL FORMULATION

2.1 INTRODUCTION

The problem of parameter estimation from a limited number of observations is of considerable interest and importance in hydrology. By late 1960's, hydrologists had been in a quandary owing to the lack of a systematic procedure for parameter identification, and most existing methods had required graphical matching.

In recent years, a great number of simulation and mathematical models are often used in analyzing the groundwater system. Most models are of parametric type in which the parameters or coefficients are not simply measurable from the physical point of view. However, these parameters can be identified by using concurrent input and output observations on the dependent variable of the governing equation along with appropriate initial and boundary conditions. These models are then used conjunctively with the surface water system for prediction and management of the integrated basin. Optimum development and management are achieved in most cases when pumping of ground water is balanced by replenishment.

The problem of parameter estimation in the groundwater aquifer system has been reported by numerous researchers. A survey of parameter identification in distributed systems governed by partial differential equations was reported by Kubrusly (35). Proposed methods may be classified into two groups: the direct approach and the indirect approach. The indirect methods depend upon the division of the inhomogeneous aquifer system into several approximately homogeneous subregions for which prior information can be used for the initial estimates of the parameters. These initial estimates are then improved iteratively until the model response is sufficiently close to that of the field observations. As a result, the indirect method is an optimization procedure in which the objective is usually the minimization of a norm of the differences between observed and calculated groundwater levels at the specified observation points.

Vemuri and Karplus (63) solved the inverse problem by using the maximum principle in conjunction with the steepest descent algorithm on a hybrid computer. The other developed methods in line with gradient techniques include those by Jacquard and Jane (30), Seinfeld (57,58), Chen and Seinfeld (16), Chen et al. (17), and Bruch et al. (13). Yeh and Tauxe (72) used quasilinearization allied with the finite difference scheme in order to solve the inverse problem. The other articles concerned with quasilinearization include Yeh (67,68), Marino and Yeh (43), and Lin and Yeh (41). Linear programming was used by Slater and Durrer (60), Yeh and Becker (71), and Coats et al. (18). Yeh (70) and Chang and Yeh (15) solved the problem by quadratic programming with a quadratic performance criterion subject to lower and upper bounds on parameters to be identified. Yeh (69) made a comparative study using five different approaches: quasi-linearization, maximum principle, gradient method, influence coefficient method and linear programming. The finite element ideas were used by Distefano and Rath (22). Yoon and Yeh (74) proposed the modified Gauss-Newton method allied with the finite elements. The mixed explicit-implicit Galerkin finite element method was used by Neuman and Narasimhan (50) and Narasimhan et al. (47).

The direct methods, such as those of Nelson (48) and Emsellem and de Marsily (23), are available if the groundwater levels can be specified on a regular mesh of grid points covering the area of interest. The direct approach treats the model parameters as dependent variables in a formal inverse boundary value problem. Frind and Pinder (24) used Galerkin's method for steady flow. A multiple objective decision process was used by Neuman (49). In actual field practice, observation wells are sparsely located in random fashion rather than regularly located; and only a limited number of wells are available. Sagar et al. (55) proposed the method of spline interpolation to fit the discrete data of observations; but the method still requires a sufficient number of the observation points to properly approximate the whole flow potential surface in the region under consideration.

In dealing with noisy data, Wilson et al. (65) proposed an approach based on the notion of a Kalman filter to permit utilization of prior information about the parameters. A nonlinear least squares method for estimating parameters in two dimensional or radial steady state groundwater motion was used by Cooley (19,20). This approach promises as an aid to establishing approximate reliability of computed parameters and predicted head distribution. The role of statistics in the determination of optimum parameter dimension with respect to modeling error was studied in considerable depth by Shah et al. (59). Neuman and Yakowitz (50) and Neuman et al. (52) used a Bayesian type of approach for estimating spatially varying aquifer transmissivities on the basis of steady state and noisy water level data utilizing a priori statistics of the aquifer system. Recently, Yeh and Yoon (73) presented a parameter identification procedure using a modified Gauss-Newton algorithm for parameter optimization and covariance analysis for estimating the reliability of the estimated parameters.

2.2 HYDROLOGICAL BACKGROUND

Water is an essential commodity to mankind, and the largest available sources of fresh water lies underground. Increased demands for water have stimulated development of underground water supplies.

The problem under consideration is that of an unsteady flow of water in an unconfined aquifer stream interaction system. Groundwater occurs in permeable geologic formulations known as aquifers, that is, formations having structures that permit appreciable water to move through them under ordinary field conditions. The word aquifer, which can be traced to its Latin origin, is a combining form of aqua, meaning water, and ferre, to bear. Hence, an aquifer, literally, is a water bearer.

The subsurface occurrence of groundwater may be divided into zones of saturation and aeration. Over most of the land masses of the earth a single zone of aeration overlies a single zone of saturation and extends upward to the ground surface, as shown in Figure 1. The saturated zone is bounded at the top by either a limiting surface of saturation or overlying impermeable strata, and extends down to underlying impermeable strata such as clay beds or bedrock. In the absence of overlying impermeable strata, the upper surface of the zone of saturation is the water table. This is defined as the surface of atmospheric pressure and would be revealed by the level at which water stands in a well penetrating the aquifer. Water occurring in the zone of saturation is commonly referred to simply as groundwater.

Aquifers may be classed as unconfined or confined, depending upon the presence or absence of a water table. An unconfined aquifer is one in which a water table serve as the upper surface of the zone of saturation. Rises and falls in the water table correspond to changes in the volume of water in storage within an aquifer. Figure 1 is an idealized section through an unconfined aquifer.

2.3 MATHEMATICAL MODEL

A one dimensional simplified but typical inverse problem,

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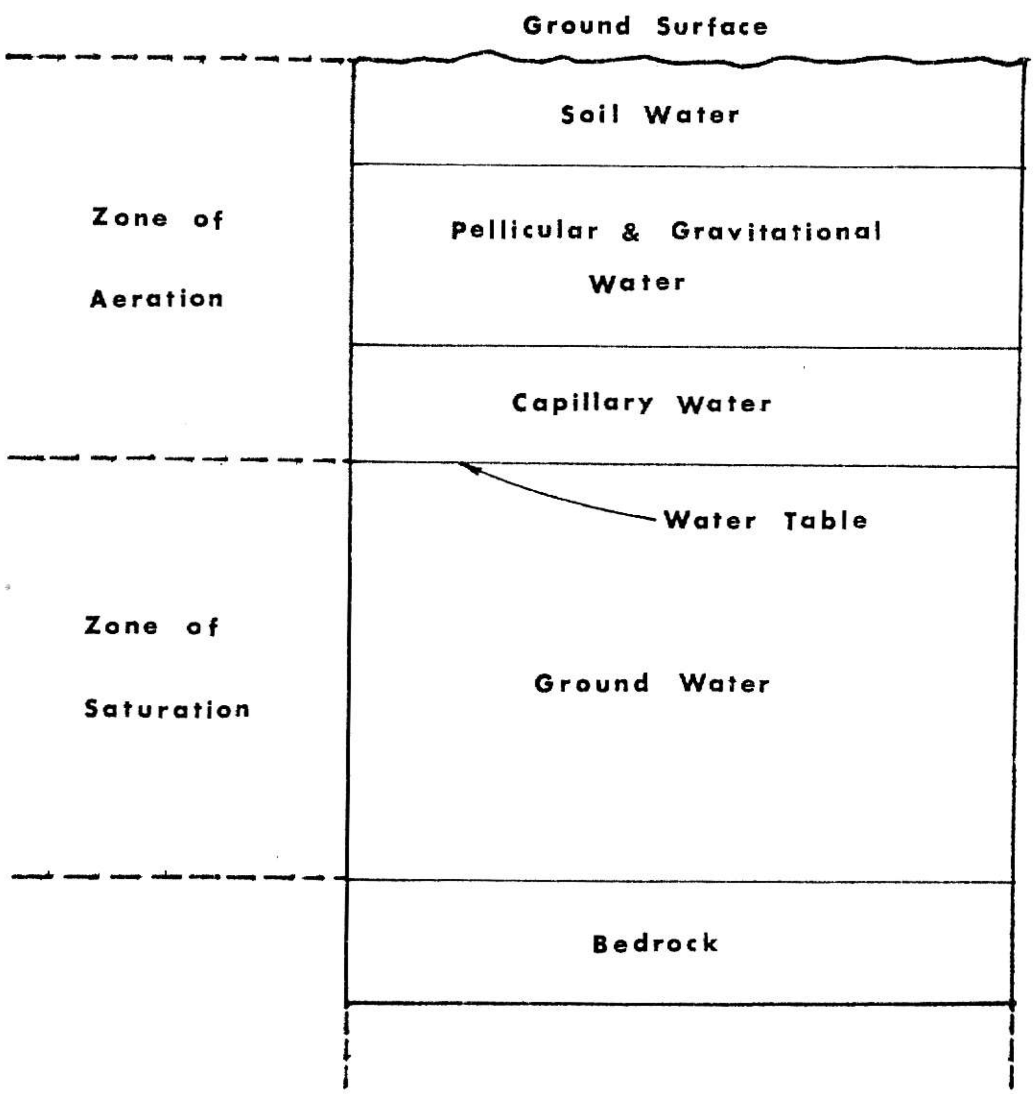

Figure 1. Division of subsurface water

governed by nonlinear partial differential equations, is analyzed. The problem under consideration is that of an unsteady flow in an unconfined aquifer stream interaction system. Figure 2 shows schematically the flow configuration of an unconfined aquifer and stream interaction system. If the curvature of the free water table is small, the Dupuit-Forchheimer concepts may be assumed to be valid. It is also assumed that the unconfined aquifer is homogeneous and isotropic.

In 1856, Henry Darcy, a French hydraulic engineer, reported a simple empirical relation based on his experiments, namely,

$$v = K \, \partial h/\partial x \qquad (2.1)$$

where v is the velocity of flow, K is the hydraulic permeability of the unconfined aquifer, x is space variable, and $\partial h/\partial x$ is the hydraulic gradient. Equation (2.1), commonly called Darcy's law, demonstrates a linear dependency between the hydraulic gradient and the velocity of flow v. Then, the flow Q through a unit width at a distance x and with a head h is

$$Q = Av = Kh \, \partial h/\partial x \qquad (2.2)$$

where A is the saturated area, which has a unit width, perpendicular to the flow; and h is the head in aquifer, a function of x and t.

The rate of change of Q with respect to x is

$$\partial Q/\partial x = K(\partial/\partial x)(h \, \partial h/\partial x). \qquad (2.3)$$

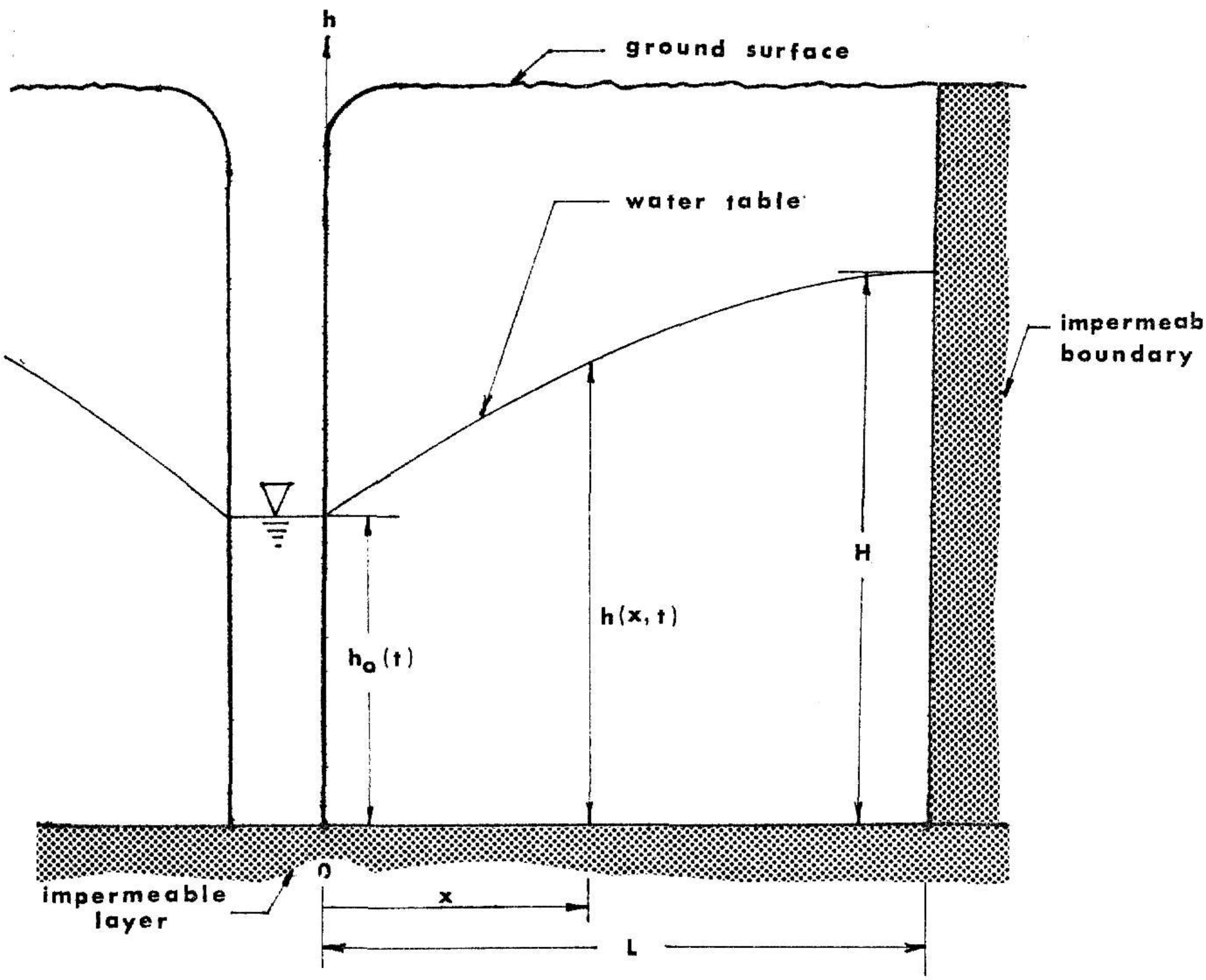

Figure 2. Unconfined aquifer and stream interaction configuration

Another expression for Q may be written in terms of the change in storage of water beyond x, with respect to time, as follows:

$$Q = \int_{x}^{\infty} du\, S'(\partial h/\partial t) \tag{2.4}$$

in which S' is the specific storage of the aquifer and t is time. The specific storage S'(dimensionless) is the drainable volume in the aquifer expressed as a ratio to the gross volume. In other words, S' is the volume of fluid instantaneously released from storage per unit bulk volume of porous medium when h is lowered by one unit.

In terms of the change of flow with respect to x, Equation (2.4) may be written as:

$$\partial Q/\partial x = S'(\partial h/\partial t). \tag{2.5}$$

By combining Equations (2.3) and (2.5), the following non-linear differential equation is obtained

$$K(\partial/\partial x)(h\, \partial h/\partial x) = S'(\partial h/\partial t) \tag{2.6}$$

subject to the following initial and boundary conditions:

$$\begin{aligned} h(x, 0) &= h(x) \\ h(0, t) &= h_0(t) \\ \partial h/\partial x \Big|_{(L,\ t)} &= 0 \end{aligned} \tag{2.7}$$

where K, h, x, S', and t are as previously defined;

h(x) = given initial condition;

$h_0(t)$ = given boundary condition;

L = maximum distance from the river to the water divide;

$\partial h/\partial x \Big|_{(L,\ t)}$ = no flow condition at x = L, equal to 0.

2.4 ANALYTICAL FORMULATION

By rearranging Equation (2.6), the governing equation can be expressed as:

$$\partial h/\partial t = (K/S')(\ \partial/\partial x\ )(\ h\ \partial h/\partial x\ ). \qquad (2.8)$$

Equation (2.8) delineates a distributed system in which the parameters are constant. To make the head and the space variable dimensionless, the following changes in variables are introduced:

$$\theta = h/H \qquad y = x/L \qquad \tau = (H/L^2)t \qquad (2.9)$$

where H is the maximum water table height. Substituting Equation (2.9) into Equation (2.8) yields

$$\partial\theta/\partial\tau = D(\ \partial/\partial y\ )(\ \theta\, \partial\theta/\partial y\ ) \qquad (2.10)$$

subject to

$$\begin{aligned} \theta(y,\ 0) &= h(x)/H \\ \theta(0,\ \tau) &= h_0(t)/H \qquad (2.11) \\ \partial\theta/\partial\tau \Big|_{(1,\ \tau)} &= 0 \end{aligned}$$

where diffusivity D = K/S'.

The inverse problem being considered is the one of determining the aquifer diffusivity, D. It is assumed that observations on θ are available at an observation well within the system. The objective is to uncover this unknown parameter along with these given observations and appropriate initial and boundary conditions.

Equation (2.10) characterizes a distributed system and can be transformed to a lumped system via a spatial discretization scheme. To minimize the truncation error introduced by the finite difference approximations, the central difference scheme is used. The goal of finite difference method is to transform the distributed equations into a set of difference equations.

The space variable y of Equation (2.10) is discretized into n equal intervals, where i = 1, 2, ..., n while the time variable τ is being kept continuous. The finite difference approximation of Equation (2.10) becomes

$$d\theta/d\tau = D\left\{\frac{1}{\Delta y}\left[\left(\frac{\theta_{i+1}+\theta_i}{2}\right)\left(\frac{\theta_{i+1}-\theta_i}{\Delta y}\right) - \left(\frac{\theta_i+\theta_{i-1}}{2}\right)\left(\frac{\theta_i-\theta_{i-1}}{\Delta y}\right)\right]\right\} \quad (2.12)$$

$$i = 1, 2, \ldots, (n-1)$$

After simplification, it reduces to

$$\dot{\theta}_i = D\,\frac{1}{2(\Delta y)^2}\left(\theta_{i+1}^2 - 2\,\theta_i^2 + \theta_{i-1}^2\right) \quad (2.13)$$

$$i = 1, 2, \ldots, (n-1)$$

where $\dot{\theta}_i = d\theta_i/d\tau$. Figure 3 shows the discretized configuration.

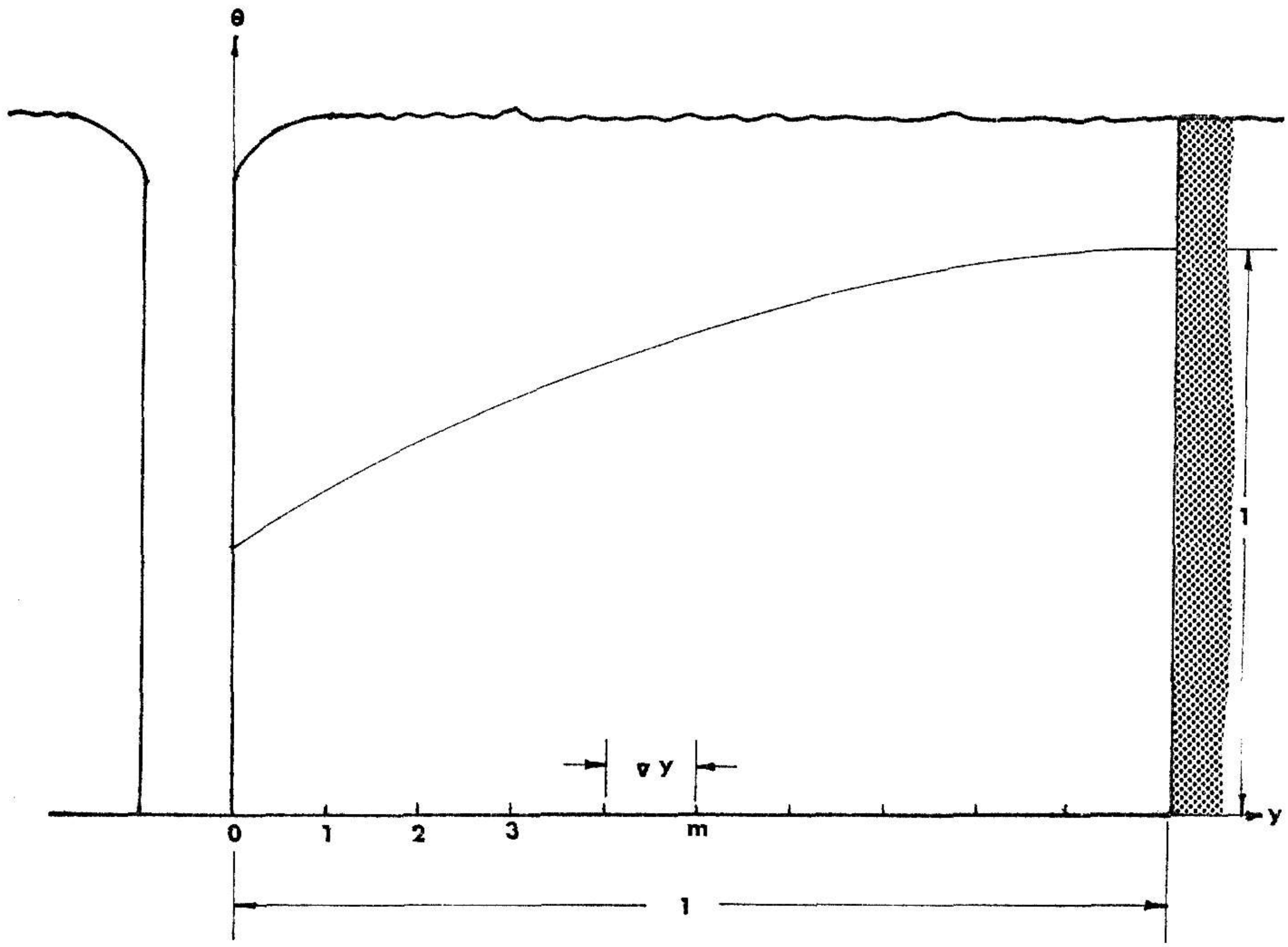

Figure 3. Finite difference approximation for the space variable y

CHAPTER 3

PARAMETER ESTIMATION BY QUASILINEARIZATION

3.1 INTRODUCTION

The quasilinearization technique which can be classified into the indirect method is introduced in this chapter. Emphasis is placed on the numerical aspects of estimation process concerning its application to the groundwater aquifer system rather than theoretical derivations.

The quasilinearization technique is essentially a generalized Newton-Raphson method for functional equations. The quasilinearization technique not only linearizes the nonlinear equation but also provides a sequence of functions which converges quadratically to the solution of the original nonlinear equation.

Yeh's study (72) will be verified by using the same guessed initial value of aquifer diffusivity. The technique will be further tested by using different value of diffusivity. The computational aspects of parameter estimation procedure is discussed in detail.

Generally, the indirect approach is an optimization procedure in which the objective is the minimization of a norm of the differences between observed value and calculated one. For the objective function, the least squares approach is introduced.

3.2 LEAST SQUARES APPROACH

Suppose that observations are made at an observation well at some distance between 0 and 1, say, at the $m^{\underline{th}}$ discretized point on the dimensionless scale, where $1 \leq m \leq (n-1)$. Thus, the dimensionless head at this point observed for various values of τ(time), say τ_1, τ_2, ..., τ_T, defined as

$\theta_m^*(\tau_j)$ = observed dimensionless head at the $m^{\underline{th}}$ discretized point at time τ_j, $j = 1, 2, \ldots, T$.

The objective is to uncover the unknown parameter D such that the solution of the nonlinear governing Equation (2.10) is in closest agreement with the observations $\theta_m^*(\tau_j)$. When the classical least squares criterion is used, the objective function is the minimization of the weighted sum of the squares of the deviations:

$$J_0 = \sum_j \left[\theta_m(\tau_j) - \theta_m^*(\tau_j) \right]^2 w_j \qquad (3.1)$$

$$j = 1, 2, \ldots, T$$

where w_j represents the weight to be assigned to each of the observations and $\sum_j (w_j/T) = 1$, $j = 1, 2, \ldots, T$.

The solutions of $\theta_m(\tau_j)$ are obtained by direct numerical integration of Equation (2.13) subject to (2.11) when some considered value is used for the parameter D.

3.3 QUASILINEARIZATION

Quasilinearization is a technique which involves solving a series of linear initial value problems such that the sequence of solutions converges to the solution of the original problem. The linearized equations serve as a means to identify the unknown parameter D.

3.3.1 LINEARIZATION

The nonlinear term in Equation (2.13) can be linearized by the use of the following expression:

$$f(u_{k+1}, v_{k+1}) = f(u_k, v_k) + (u_{k+1} - u_k)\, f_u(u_k, v_k) + (v_{k+1} - v_k)\, f_v(u_k, v_k) \tag{3.2}$$

which is obtained from Taylor's series with second and higher order terms neglected. The term $f_u(u_k, v_k)$ and $f_v(u_k, v_k)$ represent partial differentiations of $f(u_k, v_k)$ with respect to u_k and v_k, respectively. If we assume u_k and v_k are the known values and u_{k+1} and v_{k+1} are the unknowns, the right-hand side of Equation (3.2) will always be linear.

Equation (2.13) now becomes

$$\dot{\theta}_i^{k+1} = D^k \frac{1}{2(\Delta y)^2} \left(\theta_{i+1}^{k^2} - 2\, \theta_i^{k^2} + \theta_{i-1}^{k^2} \right) + (\theta_{i+1}^{k+1} - \theta_{i+1}^{k}) \left[\frac{D^k}{2(\Delta y)^2} (2\, \theta_{i+1}^{k}) \right]$$

$$+ \left(\theta_i^{k+1} - \theta_i^k \right) \left[\frac{D^k}{2(\Delta y)^2} \left(-4\, \theta_i^k\right) \right]$$

$$+ \left(\theta_{i-1}^{k+1} - \theta_{i-1}^k \right) \left[\frac{D^k}{2(\Delta y)^2} \left(2\, \theta_{i-1}^k\right) \right] \delta$$

$$+ \left(D^{k+1} - D^k \right) \left[\frac{1}{2(\Delta y)^2} \left(\theta_{i+1}^{k^2} - 2\theta_i^{k^2} + \theta_{i-1}^{k^2} \right) \right] \qquad (3.3)$$

$$i = 1, 2, 3, \ldots, (n-1)$$

$$\delta = 0 \quad \text{for} \quad i = 1$$

$$\delta = 1 \quad \text{for} \quad i \neq 1$$

subject to

$$\theta^{k+1}(y, 0) = h(x)/H$$

$$\theta^{k+1}(0, \tau) = h_0(t)/H \qquad (3.4)$$

$$\theta_n^{k+1} = \theta_{n-1}^{k+1} \qquad y = 1, \tau > 0$$

in which the superscript k+1 represents the new approximation and k denotes the previous approximation.

3.3.2 METHOD OF COMPLEMENTARY FUNCTION

The method of complementary function is used to obtain the general solution of Equation (3.3) and requires only the previous estimates of D^k and solutions of θ_i^k.

Consider a general first order differential equation

$$\frac{dy}{dx} + P(x)y = k_1F_1(x) + k_2F_2(x) \qquad (3.5)$$

where k_1 and k_2 are constants; P, F_1, and F_2 are all defined on the same real domain. Let p be a particular solution of

$$\frac{dy}{dx} + P(x)y = F_1(x) \tag{3.6}$$

Let q be a particular solution of

$$\frac{dy}{dx} + P(x)y = F_2(x) \tag{3.7}$$

Then $k_1p + k_2q$ is also a solution of Equation (3.5).

The general solution is used to obtain the new estimate of D^k and is formed by the linear combination of the particular solutions of Equation (3.3).

Rearranging Equation (3.3), one gets

$$\begin{aligned}
\dot{\theta}_i^{k+1} &- \theta_{i+1}^{k+1}\left[\frac{D^k}{2(\Delta y)^2}(2\,\theta_{i+1}^k)\right] \\
&- \theta_i^{k+1}\left[\frac{D^k}{2(\Delta y)^2}(-4\,\theta_i^k)\right] \\
&- \theta_{i-1}^{k+1}\left[\frac{D^k}{2(\Delta y)^2}(2\,\theta_{i-1}^k)\right]\cdot\delta \\
= D^{k+1}&\left[\frac{1}{2(\Delta y)^2}\left(\theta_{i+1}^{k^2} - 2\,\theta_i^{k^2} + \theta_{i-1}^{k^2}\right)\right] \\
&+ \left\{-\theta_{i+1}^k\left[\frac{D^k}{2(\Delta y)^2}(2\,\theta_{i+1}^k)\right]\right. \\
&- \theta_i^k\left[\frac{D^k}{2(\Delta y)^2}(-4\,\theta_i^k)\right] \\
&\left.- \theta_{i-1}^k\left[\frac{D^k}{2(\Delta y)^2}(2\,\theta_{i-1}^k)\right]\right\}
\end{aligned} \tag{3.8}$$

$$i = 1, 2, 3, \ldots, (n-1)$$
$$\delta = 0 \quad \text{for} \quad i = 1$$
$$\delta = 1 \quad \text{for} \quad i \neq 1$$

Thus the right-hand side of Equation (3.8) can be expressed as $D^{k+1}F_1 + F_2$. Then, the following two particular equations are obtained:

$$\dot{p}_i = p_{i+1}\left[\frac{D^k}{2(\Delta y)^2}(2\,\theta^k_{i+1})\right] + p_i\left[\frac{D^k}{2(\Delta y)^2}(-4\,\theta^k_i)\right] + p_{i-1}\left[\frac{D^k}{2(\Delta y)^2}(2\,\theta^k_{i-1})\right]\cdot\delta + \frac{1}{2(\Delta y)^2}\left(\theta^{k^2}_{i+1} - 2\,\theta^{k^2}_i + \theta^{k^2}_{i-1}\right) \tag{3.9}$$

$$i = 1, 2, 3, \ldots, (n-1)$$
$$\delta = 0 \quad \text{for} \quad i = 1$$
$$\delta = 1 \quad \text{for} \quad i \neq 1$$

subject to

$$p(y, 0) = 0$$
$$p(0, \tau) = h_0(t)/H \tag{3.10}$$
$$p_n = p_{n-1} \qquad y = 1, \tau > 0$$

and

$$\dot{q}_i = (q_{i+1} - \theta^k_{i+1})\left[\frac{D^k}{2(\Delta y)^2}(2\theta^k_{i+1})\right]$$

$$+ (q_i - \theta_i^k) \left[\frac{D^k}{2(\Delta y)^2} (-4\, \theta_i^k) \right]$$

$$+ (q_{i-1} - \theta_{i-1}^k) \left[\frac{D^k}{2(\Delta y)^2} (2\, \theta_{i-1}^k) \right] \cdot \delta \qquad (3.11)$$

$i = 1, 2, 3, \ldots, (n-1)$

$\delta = 0 \quad \text{for} \quad i = 1$

$\delta = 1 \quad \text{for} \quad i \neq 1$

subject to

$$q(y, 0) = h(x)/H$$

$$q(0, \tau) = h_0(t)/H \qquad (3.12)$$

$$q_n = q_{n-1} \quad y = 1, \tau > 0$$

Note that the initial conditions in Equations (3.10) and (3.12) are chosen in such a way that the general solutions of Equation (3.3) satisfy the given initial conditions of Equation (3.4) at $\tau = 0$.

Now, the general solution of Equation (3.3) is represented by the linear combination of these particular equations when multiplied by the appropriate constant to give

$$\theta_i^{k+1} = D^{k+1} p_i + q_i \qquad (3.13)$$

$i = 1, 2, 3, \ldots, (n-1)$

3.4 PARAMETER ESTIMATION

The general solution of the m^{th} discretized point, where observations are made, is obtained from Equation (3.13)

$$\theta_m^{k+1} = D^{k+1} p_m + q_m \tag{3.14}$$

The new estimate of D^{k+1} is still unknown. It is determined by substituting Equation (3.14) into Equation (3.1) and minimizing the resultant function,

$$J = \sum_{j=1}^{T} \left[(D^{k+1} p_m + q_m) - \theta_m^*(\tau_j) \right]^2 \cdot w_j \tag{3.15}$$

Equation (3.15) is actually the linearized form of Equation (3.1), using the linearized general solution for θ_m. It serves as a means of identifying the unknown.

The new estimate of D^{k+1} is found by equating the derivative of J with respect to D^{k+1} to zero:

$$\frac{\partial J}{\partial D^{k+1}} = 2 \sum_{j=1}^{T} \left\{ \left[(D^{k+1} p_m + q_m) - \theta_m^*(\tau_j) \right] w_j \, p_m \right\}$$

$$= 0 \tag{3.16}$$

Then, the solution of D^{k+1} is

$$D^{k+1} = \frac{\sum_{j=1}^{T} \left[\theta_m^*(\tau_j) \, p_m - q_m \, p_m \right] w_j}{\sum_{j=1}^{T} \left[p_m^2 \, w_j \right]} \tag{3.17}$$

The governing Equation (2.13) is now integrated by using this new value of D^{k+1}. The result of this integration is checked with the observations by using the objective function, Equation (3.1). If J_0 lies below the prescribed convergence criterion ϵ, the parameter estimation problem is completed. Otherwise the linearized form of the governing Equation (3.3) is numerically integrated by using the new estimates of D and θ_i. The second cycle is started by incrementing k and returning to the reevaluation of the particular solutions of Equations (3.9) and (3.11). This procedure may be repeated until satisfactory convergence is obtained.

It is now possible to present the exact procedure of the quasilinearization technique. The following basic steps are involved:

(The basic cycle starts at iteration 0, i.e., k = 0.)

STEP 1: Linearize the governing Equation (2.13) by the use of Taylor's series expansion with maintaining only the linear terms.

STEP 2: Assume a reasonable initial value of the parameter (D^0).

STEP 3: Integrate the nonlinear governing Equation (2.13) subject to Equation (3.4) by using D^0.

STEP 4: Integrate the particular Equations (3.9) and (3.11) using the results (θ_i^0) from STEP 3.

STEP 5: Solve Equation (3.17) for the new estimate of parameter D^1 using the newly obtained particular solutions from STEP 4 and the observation data at the m^{th} discretized point.

STEP 6: Integrate the governing Equation (2.13) by using D^1 in order to estimate the new θ_i^1.

STEP 7: Evaluate J_0 by using Equation (3.1) and compare with the prescribed convergence criterion ϵ.

STEP 8: If $J_0 < \epsilon$, the parameter estimation problem is completed. Otherwise, integrate the linearized governing Equation (3.3) by using D^1. Then, go to STEP 4.

Note that the best available initial estimate of parameter D should be used for STEP 2. Figure 4 shows the flow chart of computer program for the quasilinearization algorithm.

The initial parameter estimation can affect the convergence, depending on the sensitivity of the solution to that parameter. If this initial approximation is too far from the correct solution of the problem, the iteration procedure may not converge. In order to converge, this initial approximation value must be within a certain interval, which is referred to as the interval of convergence. The best remedy is to attempt another estimate of the parameter.

3.5 NUMERICAL RESULTS

To illustrate the applicability of the technique, the aquifer diffusivity D is estimated. Also of importance is the ability to calculate θ_i.

EXAMPLE 1

As a verification of Yeh's study (72), the inverse problem

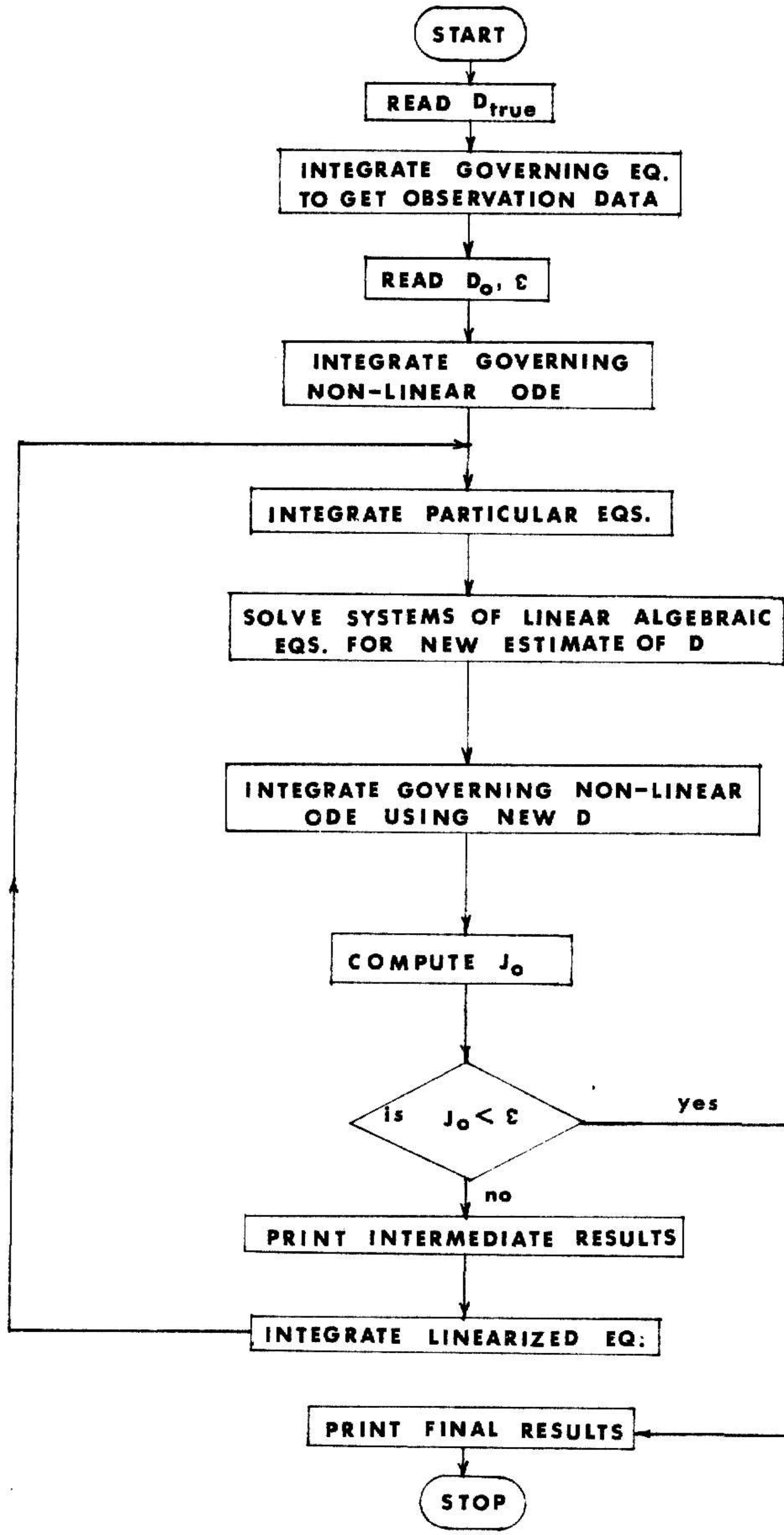

Figure 4. Flow chart of computer program for the quasi-linearization algorithm

is solved and compared with Yeh's result for the following initial and boundary conditions:

$$\begin{aligned} \theta_i(0) &= 1.0 \\ \theta_0(\tau) &= 0.5 \\ \theta_n(\tau) &= \theta_{n-1}(\tau) \end{aligned} \tag{3.18}$$

In addition, the following values are also assumed:

$$\begin{aligned} H/L^2 &= 1 \\ D &= 1 \end{aligned} \tag{3.19}$$

The observation data $\theta_i(\tau)$ are generated by integrating Equation (2.13) subject to Equation (3.18) with D = 1. Ten intervals on the space variable y were used; i. e., $\Delta y = 0.1$. The Runge-Kutta integration scheme was used with step size of $\Delta t = 0.002$. The generated observed values of the dimensionless head at the fifth discretized point are shown in Table 1. These values are used as observations in order to test the quasilinearization algorithm.

In order to test the procedure, a value of $D^0 = 0.1$ was used as the initial estimate of the aquifer diffusivity. This initial estimate is different from D = 1 by a factor of 10. Convergence criterion was set at $\epsilon = 10^{-6}$. Convergence was obtained in only four iterations. Comparison of the present results of successive approximations with Yeh's results is shown in Table 2. The objective function J_0 is also compared by

Table 1. Observed values of the dimensionless head at the fifth discretized point for D = 1.0

j	τ_j	$\theta_5^*(\tau_j)$ Yeh's @	$\theta_5^*(\tau_j)$ Present Work
1	0	1.00000	1.00000
2	0.1	0.90518	0.90489
3	0.2	0.82802	0.82796
4	0.3	0.77215	0.77211
5	0.4	0.72803	0.72799
6	0.5	0.69229	0.69225
7	0.6	0.66296	0.66293
8	0.7	0.63867	0.63866
9	0.8	0.61842	0.61840
10	0.9	0.60142	0.60140
11	1.0	0.58707	0.58706

@ Yeh, W. W-G., and Tauxe, G. W., Water Resources Research, 7(4), 955, 1971.

Table 2. Comparison of the numerical results of successive approximations at the final iteration for D = 1.0

	Yeh's @		Present Work	
	Final(fourth)	Observations	Final(fourth)	Observations
D	1.00102	1.00000	1.00020	1.00000
$\theta_5(0)$	1.00000	1.00000	1.00000	1.00000
$\theta_5(0.1)$	0.90506	0.90518	0.90487	0.90489
$\theta_5(0.2)$	0.82789	0.82802	0.82793	0.82796
$\theta_5(0.3)$	0.77200	0.77215	0.77207	0.77211
$\theta_5(0.4)$	0.72787	0.72803	0.72795	0.72799
$\theta_5(0.5)$	0.69213	0.69229	0.69222	0.69225
$\theta_5(0.6)$	0.66280	0.66296	0.66290	0.66293
$\theta_5(0.7)$	0.63852	0.63867	0.63862	0.63866
$\theta_5(0.8)$	0.61827	0.61842	0.61837	0.61840
$\theta_5(0.9)$	0.60127	0.60142	0.60137	0.60140
$\theta_5(1.0)$	0.58694	0.58707	0.58703	0.58706
J_0	2.2010×10^{-7}		1.1632×10^{-8}	

@ Yeh, W. W-G., and Tauxe, G. W., Water Resources Research, 7(4), 955, 1971.

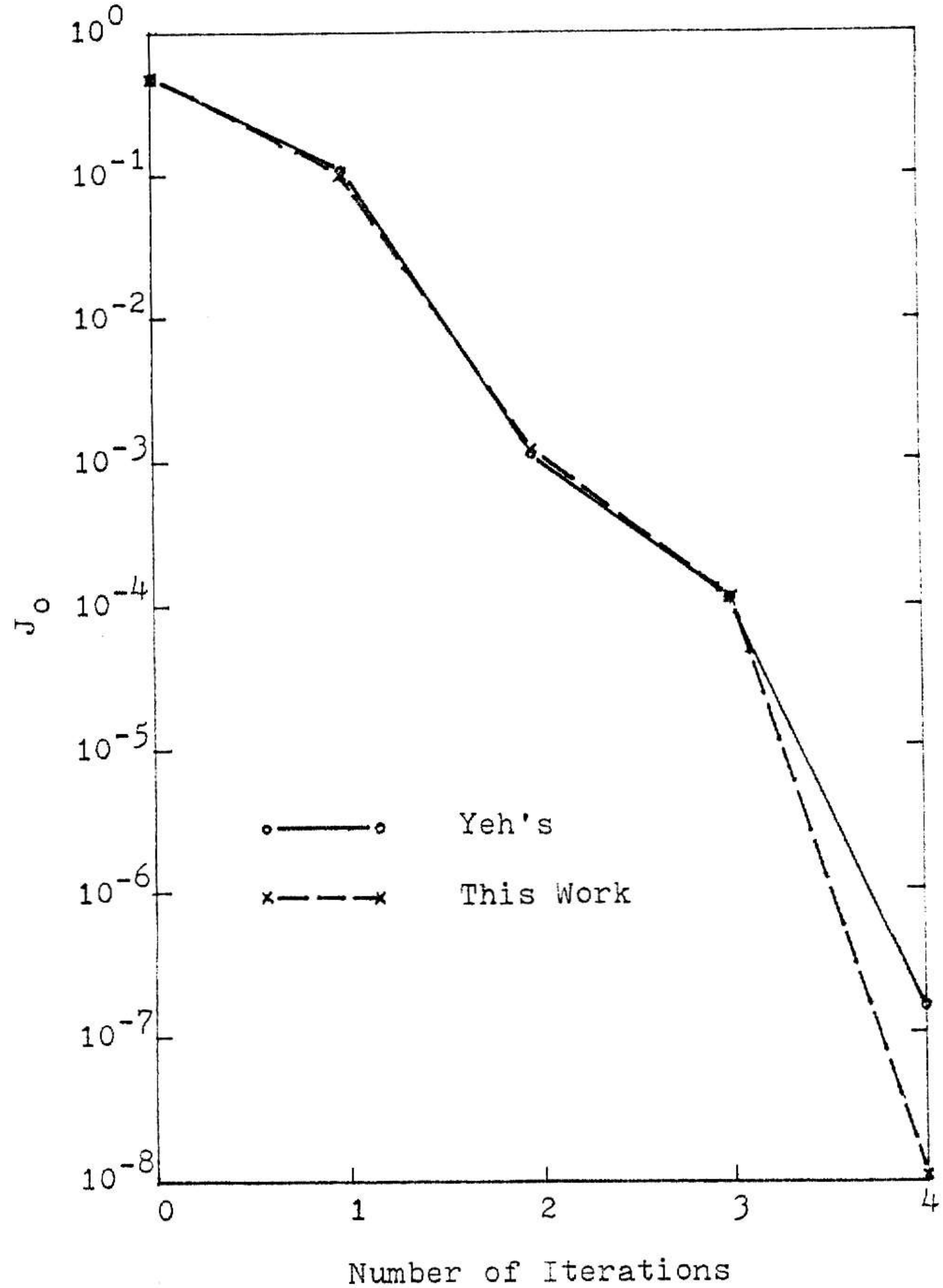

Figure 5. J_0 vs. number of iterations for D = 1.0

plotting it in Figure 5.

EXAMPLE 2

For further confirmation, D = 0.1 was attempted. The same initial and boundary conditions, $H/L^2 = 1$, and $\Delta y = 0.1$ of EXAMPLE 1 were used. The Runge-Kutta method was used again with $\Delta t = 0.002$. Table 3 shows the generated observation data of the dimensionless head.

The procedure is tested with the initial estimates of the aquifer diffusivity $D^0 = 0.03$ and 0.3, respectively. Convergence criterion was set at $\epsilon = 10^{-7}$. Convergence was obtained within only three iterations in both cases. Tables 4 and 5 show the results of successive approximations corresponding to $D^0 = 0.03$ and 0.3, respectively. The J_0 functions are plotted in Figure 6. It is shown that the quadratic convergence is obvious.

3.6 DISCUSSION

The technique of quasilinearization has been successfully applied to parameter estimation in an unconfined aquifer system. The observation data were generated using the assumed value of aquifer diffusivity. Yeh's study (72) was then verified by using the same initial estimate of diffusivity. The technique was further tested by choosing different value and different initial estimates of diffusivity. In every case, the parameter converged in less than five iterations. The least squares criterion was used for the objective function. In general, it can be said that as long as the initial approximations are

Table 3. Observed values of the dimensionless head $\Theta_i(\tau)$ for D = 0.1

i	τ = 0.0	τ = 0.1	τ = 0.2	τ = 0.3	τ = 0.4	τ = 0.5	τ = 0.6	τ = 0.7	τ = 0.8	τ = 0.9	τ = 1.0
0	1.00000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000	0.50000
1	1.00000	0.81323	0.74816	0.71286	0.68982	0.67321	0.66048	0.65031	0.64192	0.63485	0.62877
2	1.00000	0.93963	0.88257	0.84315	0.81439	0.79226	0.77453	0.75990	0.74753	0.73689	0.72758
3	1.00000	0.98393	0.95102	0.92045	0.89481	0.87340	0.85529	0.83976	0.82624	0.81432	0.80369
4	1.00000	0.99648	0.98198	0.96303	0.94414	0.92668	0.91090	0.89670	0.88387	0.87223	0.86158
5	1.00000	0.99935	0.99418	0.98437	0.97241	0.95990	0.94764	0.93593	0.92487	0.91444	0.90461
6	1.00000	0.99990	0.99834	0.99401	0.98737	0.97937	0.97071	0.96181	0.95291	0.94413	0.93552
7	1.00000	0.99999	0.99958	0.99791	0.99464	0.98999	0.98431	0.97793	0.97108	0.96393	0.95659
8	1.00000	1.00000	0.99990	0.99933	0.99783	0.99526	0.99163	0.98708	0.98179	0.97591	0.96959
9	1.00000	1.00000	0.99998	0.99976	0.99899	0.99737	0.99476	0.99117	0.98671	0.98153	0.97577
10	1.00000	1.00000	0.99998	0.99976	0.99899	0.99737	0.99476	0.99117	0.98671	0.98153	0.97577

Table 4. Results of successive approximations with $D^0 = 0.03$ for $D = 0.1$

	Zero	First	Second	Third	Observations
D	0.03000	0.11564	0.10167	0.10002	0.10000
$\theta_5(0)$	1.00000	1.00000	1.00000	1.00000	1.00000
$\theta_5(0.1)$	1.00000	0.99893	0.99932	0.99935	0.99935
$\theta_5(0.2)$	0.99991	0.99149	0.99391	0.99417	0.99418
$\theta_5(0.3)$	0.99956	0.97891	0.98381	0.98437	0.98437
$\theta_5(0.4)$	0.99877	0.96459	0.97158	0.97239	0.97241
$\theta_5(0.5)$	0.99747	0.95028	0.95887	0.95989	0.95990
$\theta_5(0.6)$	0.99564	0.93664	0.94644	0.94762	0.94764
$\theta_5(0.7)$	0.99334	0.92385	0.93460	0.93591	0.93593
$\theta_5(0.8)$	0.99064	0.91192	0.92344	0.92485	0.92487
$\theta_5(0.9)$	0.98762	0.90076	0.91293	0.91442	0.91444
$\theta_5(1.0)$	0.98435	0.89028	0.90302	0.90458	0.90461
J_0	2.4011×10^{-2}	1.0183×10^{-3}	1.2216×10^{-5}	2.4707×10^{-9}	-

Table 5. Results of successive approximations with $D^0 = 0.3$ for $D = 0.1$

	Zero	First	Second	Third	Observations
D	0.30000	0.04306	0.09874	0.10000	0.10000
$\theta_5(0)$	1.00000	1.00000	1.00000	1.00000	1.00000
$\theta_5(0.1)$	0.98445	0.99998	0.99938	0.99935	0.99935
$\theta_5(0.2)$	0.94772	0.99963	0.99437	0.99418	0.99418
$\theta_5(0.3)$	0.91451	0.99843	0.98480	0.98437	0.98437
$\theta_5(0.4)$	0.88654	0.99617	0.97303	0.97241	0.97241
$\theta_5(0.5)$	0.86239	0.99290	0.96069	0.95990	0.95990
$\theta_5(0.6)$	0.84095	0.98883	0.94885	0.94764	0.94764
$\theta_5(0.7)$	0.82154	0.98420	0.93694	0.93593	0.93593
$\theta_5(0.8)$	0.80374	0.97918	0.92596	0.92487	0.92487
$\theta_5(0.9)$	0.78728	0.97393	0.91560	0.91444	0.91444
$\theta_5(1.0)$	0.77199	0.96857	0.90582	0.90461	0.90461
J_0	$9.7036\text{x}10^{-2}$	$1.6488\text{x}10^{-2}$	$7.0846\text{x}10^{-6}$	$3.3920\text{x}10^{-11}$	-

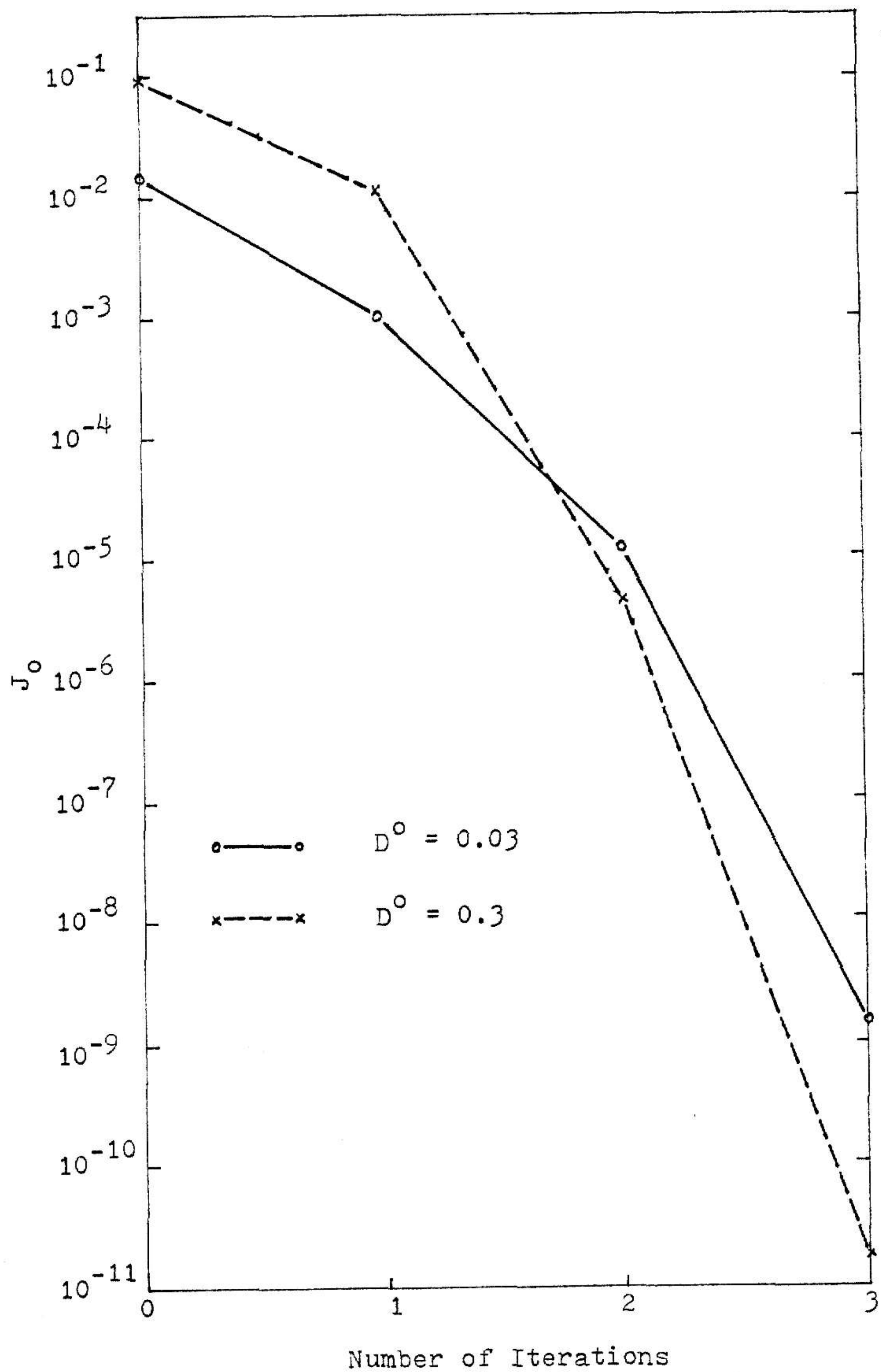

Figure 6. J_0 vs. number of iterations for D = 0.1

within the interval of convergence, the initial estimates converge to the assumed value of parameter within three to seven iterations.

No disturbances on the observation data have been introduced. However, observations are usually corrupted by instrumentation or human errors in actual field measurement. It will be an interesting problem to find this effect on parameter estimation as well as the ability of the procedure in seeking to uncover the unknowns.

CHAPTER 4

STATE AND PARAMETER ESTIMATION BY INVARIANT IMBEDDING

4.1 INTRODUCTION

The real birth of the method of invariant imbedding, originated in the work of Ambarzumian (1,2) and Chandrasekhar (14), started with the paper of Bellman and Kalaba (5) in 1956. In fact, it was Bellman who coined the present name of "the principle of invariant imbedding".

This method has been found extremely useful in various fields of physics and engineering. Chief among them are applications in neutron transport theory (10,66), radiative transfer (9,10,14), random walk and scattering (6), wave propagation (6,7), rarefied gas dynamics (3), Hamilton's equation of motion (8), and the flow in chemical reactors (38). A fairly complete bibliography can be found in the books by Lee (38), Meyer (44), and Scott (56).

The theory of invariant imbedding enables the transformation of boundary value problems into initial value problems by introducing new state variable and imbedding a particular problem in a family of analogous problems.

In this chapter, emphasis will be placed on the use of the concept of invariant imbedding as a computational tool. More theoretical formulations andanalytical applications will not be discussed because of its thorough coverage in the books mentioned and in the large number of works reported in the literature.

In essence, the sequential estimation of system parameters is nothing more or less than a problem of nonlinear filtering. The method of invariant imbedding is developed and applied to the two-point boundary value problem of parameter estimation.

4.2 NONLINEAR FILTERING AND ESTIMATION

The concept of invariant imbedding can be applied to derive some useful results in the theory of nonlinear filtering and estimation. The problem treated in the present work is essentially an extension of the well-known linear prediction problem which was discussed by Kalman and Bucy (33).

Since the invariant imbedding approach is different from the usual classical one, several advantages can be obtained (38). First, this approach is applicable to a variety of nonlinear problems. Second, in contrast to the nonsequential estimation scheme resulting from the usual classical approach, the estimator equations obtained by invariant imbedding are sequential estimators. In the nonsequential case, each time additional output data are received, the entire algorithm must be repeated from time $t = 0$ to the value of t_f to which the final data point corresponds. In the sequential case, it is desirable to continually update the state estimates from measurements or observations, and real time implementation necessitates a sequential scheme.

No statistical assumptions are made concerning the disturbances or measurement errors. For most practical problems, the determination of valid statistical data concerning these disturbances is a difficult problem in itself. The generally used least squares criterion is used to obtain the optimal estimates. If valid statistic data concerning the disturbances are available, then this criterion will not necessarily be the best one.

4.2.1 ESTIMATION PROBLEM

In general, there are two kinds of estimation problem concerning noises or disturbances involved in the experimental observations. They are;

1. The estimation of state variables and parameters with measurement errors only,
2. The same problem with both measurement errors and unknown disturbance inputs.

In the present work, the case of 'measurement errors only' is discussed.

Consider a distributed parameter system whose dynamic behavior can be represented by the nonlinear vector equation

$$\frac{d\underset{\sim}{x}}{dt} = \underset{\sim}{f}(\underset{\sim}{x},\ t) \tag{4.1}$$

where $\underset{\sim}{x}$ and $\underset{\sim}{f}$, known function, are N-dimensional vectors with components x_1, x_2, ..., x_N and f_1, f_2, ..., f_N, respectively. The problem now is to estimate state variables of the system, $\underset{\sim}{x}$. Because of the presence of disturbances or measurement errors, the observed states $\underset{\sim}{z}$ of the system do not represent the true states. Let

$$\underset{\sim}{z}(t) = \underset{\sim}{x}(t) + (\text{observation or measurement errors}) \qquad (4.2)$$

In actual situations, it is assumed that not all the state functions can be measured and some of the state functions can be measured only in certain combinations with other variables. Thus

$$\underset{\sim}{z}(t) = \underset{\sim}{h}(\underset{\sim}{x}, t) + (\text{observation or measurement errors}) \qquad (4.3)$$

where $\underset{\sim}{z}$ and $\underset{\sim}{h}$ are n-dimensional vectors with components z_1, z_2, ..., z_n and h_1, h_2, ..., h_n, respectively. The number n represents the number of measurable quantities and $n \leq N$.

When the classical least squares criterion is introduced, the actual problem now is to estimate the current states of the system at t_f, such that the following integral is minimized

$$J = \int_0^{t_f} \sum_{j=1}^{n} \left[z_j(t) - h_j(\underset{\sim}{x}, t) \right]^2 dt \qquad (4.4)$$

where t_f denotes the present time and z_j are the measured or observed functions with $0 \leq t \leq t_f$. In other words, based on the observation $\underset{\sim}{z}(t)$, $0 \leq t \leq t_f$, estimate the N conditions

$$\underset{\sim}{x}(t_f) = \underset{\sim}{c} \qquad (4.5)$$

for Equation (4.1) such that Equation (4.4) is minimized. The components of vector $\underset{\sim}{c}$ are c_1, c_2, ..., c_N. Functions h_j are evaluated on the interval $0 \leq t \leq t_f$ by using the values of $\underset{\sim}{x}$

obtained from Equation (4.1).

4.2.2 INVARIANT IMBEDDING

Let us define a new variable, $y(t)$,

$$y(t) = \int_0^t \sum_{j=1}^{n} \left[z_j(t) - h_j(\underset{\sim}{x}, t) \right]^2 dt \tag{4.6}$$

The integral Equation (4.4) can be written as

$$\frac{dy}{dt} = \sum_{j=1}^{n} \left[z_j(t) - h_j(\underset{\sim}{x}, t) \right]^2 \tag{4.7}$$

$$y(t_f) = J \tag{4.8}$$

The differential equations to be considered now are Equations (4.1) and (4.7). If the final condition (4.5) is considered as a known condition, the missing final condition is $y(t_f)$. Consider the family of problems with final points, a:

$$\underset{\sim}{x}(a) = \underset{\sim}{c} \tag{4.9}$$

with $0 \leq t \leq a$. In other words, the missing final condition, $y(t_f)$, is to be obtained by considering a family of processes with different final points, a. If we define

$r(\underset{\sim}{c}, a)$ = the missing final condition for the system represented by Equations (4.1), (4.7), and (4.9) where the process ends at $t = a$ with $\underset{\sim}{x}(a) = \underset{\sim}{c}$

then

$$y(a) = r(\underset{\sim}{c}, a) \tag{4.10}$$

Now, the invariant imbedding equation for the missing final condition can be obtained:

$$(\partial/\partial a)\left[r(\underset{\sim}{c}, a)\right] + \sum_{i=1}^{N} f_i(\underset{\sim}{c}, a)(\partial/\partial c_i)\left[r(\underset{\sim}{c}, a)\right]$$

$$= \sum_{i=1}^{n}\left[z_j(a) - h_j(\underset{\sim}{c}, a)\right]^2 \tag{4.11}$$

4.2.3 <u>ESTIMATOR EQUATION</u>

By introducing $\underset{\sim}{e}(a)$ as the optimal estimate of $\underset{\sim}{c}$ and manipulating the invariant imbedding Equation (4.11), the following sequential estimator equations are obtained:

$$\frac{d\underset{\sim}{e}}{da} = \underset{\sim}{f}(\underset{\sim}{e}, a) + \underset{\sim}{q}(a)\left[\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)\right]^T\left[\underset{\sim}{z}(a) - \underset{\sim}{h}(\underset{\sim}{e}, a)\right] \tag{4.12}$$

$$\frac{d\underset{\sim}{q}}{da} = \underset{\sim}{f}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)\,\underset{\sim}{q}(a) + \underset{\sim}{q}(a)\left[\underset{\sim}{f}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)\right]^T$$
$$+ \underset{\sim}{q}(a)\left\{\underset{\sim}{h}_{\underset{\sim}{e}\underset{\sim}{e}}(\underset{\sim}{e}, a)\left[\underset{\sim}{z}(a) - \underset{\sim}{h}(\underset{\sim}{e}, a)\right]\right\}\underset{\sim}{q}(a)$$
$$- \underset{\sim}{q}(a)\left[\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)\right]^T\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e}, a)\,\underset{\sim}{q}(a) \tag{4.13}$$

in which

a = final value of independent variable t,

$\underset{\sim}{e}$ = optimal estimates of $\underset{\sim}{c}$,

$\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e}, a) = (\partial/\partial\underset{\sim}{e})\left[\underset{\sim}{h}(\underset{\sim}{e}, a)\right]$,

$$\underset{\sim}{h}_{\underset{\sim}{e}\underset{\sim}{e}}(\underset{\sim}{e},\ a) = (\partial/\partial\underset{\sim}{e})\left[\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e},\ a)\right],$$

$$\underset{\sim}{q} = \text{weighting functions.} \tag{4.14}$$

The symbol $[\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e},\ a)]^T$ refers to the transpose of the matrix $\underset{\sim}{h}_{\underset{\sim}{e}}(\underset{\sim}{e},\ a)$. Note that Equation (4.12) represents N differential equations and Equation (4.13) represents N^2 differential equations.

The above estimator equations were originally obtained by Bellman et al. (11), and by Detchmendy and Sridhar (21) except for one additional term. The detailed derivation of these estimator equations can be found in Lee (38).

4.3 ESTIMATION OF STATE AND PARAMETER

In order ro illustrate the nonlinear filtering and estimation with invariant imbedding approach, the Example 2 solved in Section 3.5 is considered again. In the nonlinear governing Equation (2.13) with the initial and boundary conditions (2.11), both of the state θ_i and the parameter D are to be estimated. In addition to Equation (2.13), we can establish the following differential equation for D by considering D as a dependent variable and as a function of τ;

$$\frac{dD}{d\tau} = 0 \tag{4.15}$$

Now, the estimation of state θ_i and parameter D can be approached by the theory of nonlinear filtering and estimation which has been presented in Section 4.2.

The generated observed values of Table 3 are used again as measurements. For simplicity, it is assumed that no noises are involed.

The system of equations corresponding to Equation (4.1) are Equations (2.13) and (4.15) with N = 10 and n = 9. The unknown parameter D can be considered as part of the state of the system; and the estimator equations can be obtained from Equations (4.12) and (4.13) with

$$\underset{\sim}{e}(a) = \begin{bmatrix} e_1 \\ e_2 \\ \cdot \\ \cdot \\ \cdot \\ e_{10} \end{bmatrix}_{10x1}, \tag{4.16a}$$

$$\underset{\sim}{f}(\underset{\sim}{e}, a) = \begin{bmatrix} e_{10} \dfrac{1}{2(\Delta y)^2} (e_2^2 - 2e_1^2 + e_0^2) \\ e_{10} \dfrac{1}{2(\Delta y)^2} (e_3^2 - 2e_2^2 + e_1^2) \\ \cdot \\ \cdot \\ \cdot \\ e_{10} \dfrac{1}{2(\Delta y)^2} (- e_9^2 + e_8^2) \\ 0 \end{bmatrix}_{10x1}, \tag{4.16b}$$

$$\underset{\sim}{h}(\underset{\sim}{e}, a) = \begin{bmatrix} e_1 \\ e_2 \\ \cdot \\ \cdot \\ \cdot \\ e_9 \end{bmatrix}_{9x1}, \tag{4.16c}$$

$$\underset{\sim}{z}(a) = \begin{bmatrix} \theta_1^*(a) \\ \theta_2^*(a) \\ \cdot \\ \cdot \\ \cdot \\ \theta_9^*(a) \end{bmatrix}_{9x1}, \tag{4.16d}$$

and

$$\underset{\sim}{q}(a) = \begin{bmatrix} q_{11} & q_{12} & \cdot\ \cdot\ \cdot & q_{1\underline{10}} \\ q_{21} & q_{22} & \cdot\ \cdot\ \cdot & q_{2\underline{10}} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ q_{\underline{10}1} & q_{\underline{10}2} & \cdot\ \cdot\ \cdot & q_{\underline{10}\,\underline{10}} \end{bmatrix}_{10x10}, \tag{4.16e}$$

where

e_0 = optimal estimate of θ_0 which is determined from the initial and boundary conditions,

e_1 = optimal estimate of θ_1,

e_2 = optimal estimate of θ_2,

.

.

.

e_9 = optimal estimate of θ_9,

e_{10} = optimal estimate of D.

The desired estimator equations are:

$$\begin{bmatrix} \dot{e}_1 \\ \dot{e}_2 \\ \dot{e}_3 \\ \dot{e}_4 \\ \dot{e}_5 \\ \dot{e}_6 \\ \dot{e}_7 \\ \dot{e}_8 \\ \dot{e}_9 \\ \dot{e}_{10} \end{bmatrix} = \underset{\sim}{f}(\underset{\sim}{e}, a) + \underset{\sim}{q}(a) \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}_{10x9} \begin{bmatrix} \theta_1^*(a) - e_1 \\ \theta_2^*(a) - e_2 \\ \theta_3^*(a) - e_3 \\ \theta_4^*(a) - e_4 \\ \theta_5^*(a) - e_5 \\ \theta_6^*(a) - e_6 \\ \theta_7^*(a) - e_7 \\ \theta_8^*(a) - e_8 \\ \theta_9^*(a) - e_9 \end{bmatrix}_{9x1} ; \qquad (4.17a)$$

and if we let $A = \dfrac{e_{10}}{2(\Delta y)^2}$,

$$\dot{\underset{\sim}{q}}(a) = \begin{bmatrix} A(-4e_1) & A(2e_2) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{A}{e_{10}}(e_2^{\,2}-2e_1^{\,2}+e_0^{\,2}) \\ A(2e_1) & A(-4e_2) & A(2e_3) & 0 & 0 & 0 & 0 & 0 & 0 & \frac{A}{e_{10}}(e_3^{\,2}-2e_2^{\,2}+e_1^{\,2}) \\ 0 & A(2e_2) & A(-4e_3) & A(2e_4) & 0 & 0 & 0 & 0 & 0 & \frac{A}{e_{10}}(e_4^{\,2}-2e_3^{\,2}+e_2^{\,2}) \\ 0 & 0 & A(2e_3) & A(-4e_4) & A(2e_5) & 0 & 0 & 0 & 0 & \frac{A}{e_{10}}(e_5^{\,2}-2e_4^{\,2}+e_3^{\,2}) \\ 0 & 0 & 0 & A(2e_4) & A(-4e_5) & A(2e_6) & 0 & 0 & 0 & \frac{A}{e_{10}}(e_6^{\,2}-2e_5^{\,2}+e_4^{\,2}) \\ 0 & 0 & 0 & 0 & A(2e_5) & A(-4e_6) & A(2e_7) & 0 & 0 & \frac{A}{e_{10}}(e_7^{\,2}-2e_6^{\,2}+e_5^{\,2}) \\ 0 & 0 & 0 & 0 & 0 & A(2e_6) & A(-4e_7) & A(2e_8) & 0 & \frac{A}{e_{10}}(e_8^{\,2}-2e_7^{\,2}+e_6^{\,2}) \\ 0 & 0 & 0 & 0 & 0 & 0 & A(2e_7) & A(-4e_8) & A(2e_9) & \frac{A}{e_{10}}(e_9^{\,2}-2e_8^{\,2}+e_7^{\,2}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & A(2e_8) & A(-2e_9) & \frac{A}{e_{10}}(-e_9^{\,2}+e_8^{\,2}) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}_{10\times 10} \underset{\sim}{q}(a)$$

$$
+\,\underset{\sim}{q}(a)\begin{bmatrix}
A(-4e_1) & A(2e_1) & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
A(2e_2) & A(-4e_2) & A(2e_2) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & A(2e_3) & A(-4e_3) & A(2e_3) & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & A(2e_4) & A(-4e_4) & A(2e_4) & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & A(2e_5) & A(-4e_5) & A(2e_5) & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & A(2e_6) & A(-4e_6) & A(2e_6) & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & A(2e_7) & A(-4e_7) & A(2e_7) & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & A(2e_8) & A(-4e_8) & A(2e_8) & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & A(2e_9) & A(-2e_9) & 0 \\
\frac{A}{e_{10}}(e_2^2 -2e_1^2 + e_0^2) & \frac{A}{e_{10}}(e_3^2 -2e_2^2 + e_1^2) & \frac{A}{e_{10}}(e_4^2 -2e_3^2 + e_2^2) & \frac{A}{e_{10}}(e_5^2 -2e_4^2 + e_3^2) & \frac{A}{e_{10}}(e_6^2 -2e_5^2 + e_4^2) & \frac{A}{e_{10}}(e_7^2 -2e_6^2 + e_5^2) & \frac{A}{e_{10}}(e_8^2 -2e_7^2 + e_6^2) & \frac{A}{e_{10}}(e_9^2 -2e_8^2 + e_7^2) & \frac{A}{e_{10}}(-e_9^2 + e_8^2) & 0
\end{bmatrix}_{10\mathrm{x}10}
$$

$$+ \underset{\sim}{Q} - \underset{\sim}{q}(a) \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}_{10\text{x}9} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}_{9\text{x}10} \qquad (4.17\text{b})$$

where $\underset{\sim}{0}$ represents the null matrix and $\dot{\underset{\sim}{q}}(a)$ is a 10x10 dimensional matrix. Equations (4.17a) and (4.17b) represent 110 simultaneous differential equations. They can be integrated to obtain the best estimates of θ_1, θ_2, ..., θ_9, and D with a set of assumed initial conditions. In addition, it is also an interesting problem to investigate the influence of the weighting function $\underset{\sim}{q}(a)$ with various different initial values.

4.4 NUMERICAL RESULTS

In order to test the effectiveness of the estimator Equations (4.17a) and (4.17b), numerical experiments were carried out. The Runge-Kutta integration scheme with time step $\Delta t = 0.002$ was used throughout this work. The same observation data for D = 0.1 in Table 3 were used.

EXAMPLE 1

The initial conditions assumed are

$$\underset{\sim}{e}(0) = \begin{bmatrix} \theta_1^*(0) \\ \theta_2^*(0) \\ \vdots \\ \theta_9^*(0) \\ e_{10}(0) \end{bmatrix}, \tag{4.18a}$$

$$\underset{\sim}{q}(0) = \begin{bmatrix} S & 0 & . & . & . & 0 & 0 \\ 0 & S & . & . & . & 0 & 0 \\ \vdots & \vdots & & & & \vdots & \vdots \\ 0 & 0 & . & . & . & S & 0 \\ 0 & 0 & . & . & . & 0 & S \end{bmatrix} \tag{4.18b}$$

where S = 600 and $\theta_i^*(0)$ represent the measurements at $\tau = 0$. Note that $e_{10}(0)$ is the initial estimate of D. The following various different values for $e_{10}(0)$ were used.

$$e_{10}(0) = (0.01),\ (0.1),\ (0.5),\ (0.8),\ (1.0) \tag{4.19}$$

Numerical integrations were performed for each $e_{10}(0)$ of (4.19) with the other $\underset{\sim}{e}(0)$ components unchanged. The results of the estimated state at the fifth grid point $\theta_5(\tau)$ and the estimated aquifer diffusivity D are shown in Figure 7 and 8, respectively. It is shown that the closer values to D = 0.1 give faster convergence rate and better accuracy.

EXAMPLE 2

The following initial guesses with Equations (4.18a) and (4.18b) were used in order to find the effect of the diagonal terms of $\underset{\sim}{q}(0)$

$$e_{10}(0) = (0.01), \tag{4.20a}$$

$$S = (10),\ (100),\ (400),\ (800) \tag{4.20b}$$

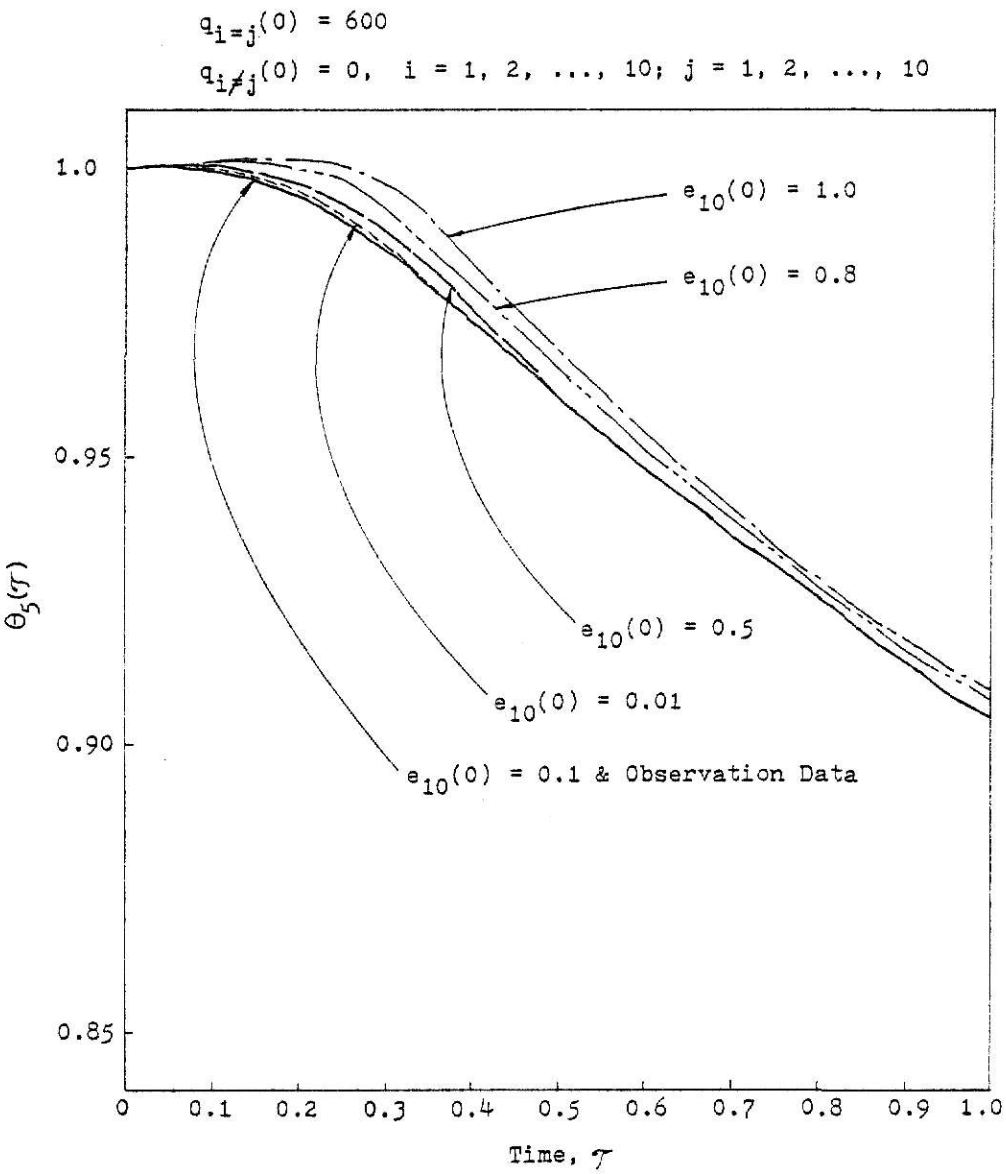

Figure 7. Estimated state $\theta_5(\tau)$ as a function of $e_{10}(0)$

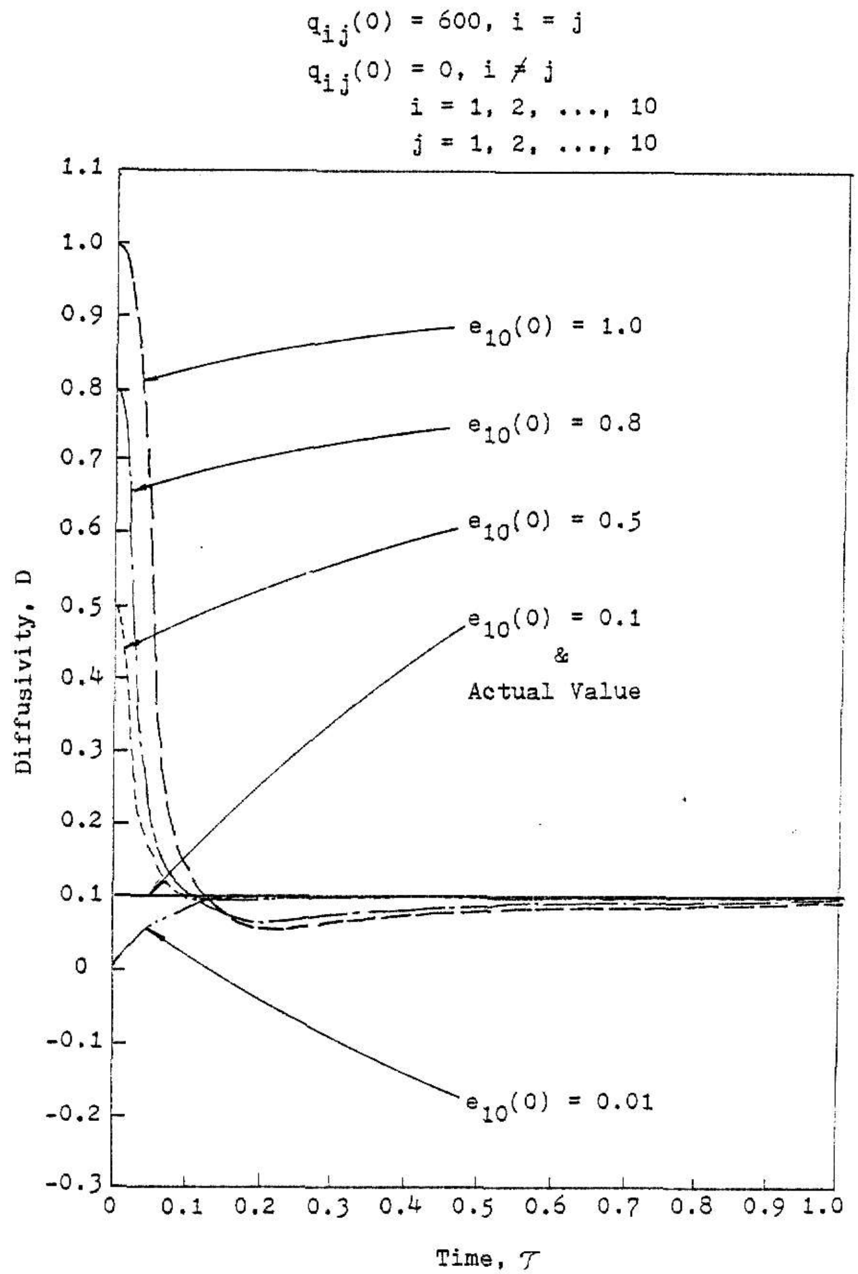

Figure 8. Estimated parameter D as a function of $e_{10}(0)$

in which the other elements of Equations (4.18a) and (4.18b) remain the same. The results of the estimated $\theta_5(\tau)$ and D are shown in Figures 9 and 10, respectively. It is observed that the estimated values of $\theta_5(\tau)$ and D approach the correct values more rapidly as the guessed value of the diagonal terms of $\underset{\sim}{q}(0)$ increases. However, when S = 900, the solutions diverged.

EXAMPLE 3

In order to test further the influence of $\underset{\sim}{q}(0)$, the following initial values in Equations (4.18a) and (4.18b) were used

$$e_{10}(0) = (0.5), \tag{4.21a}$$

$$S = (10), (100), (400), (700) \tag{4.21b}$$

while the other components were unchanged. Numerical integrations were performed again for each S value. Figures 11 and 12 show the results of the estimated $\theta_5(\tau)$ and D, respectively. As can be seen that the convergence rates are much improved with the higher values of the diagonal terms of $\underset{\sim}{q}(0)$. However, when the values of the diagonal terms were too high such as S = 800, the solutions diverged.

EXAMPLE 4

For further investigation of the influence of the diagonal terms of $\underset{\sim}{q}(0)$, the initial conditions used were

$$e_{10}(0) = (1.0), \tag{4.22a}$$

$$S = (10), (100), (400), (600) \tag{4.22b}$$

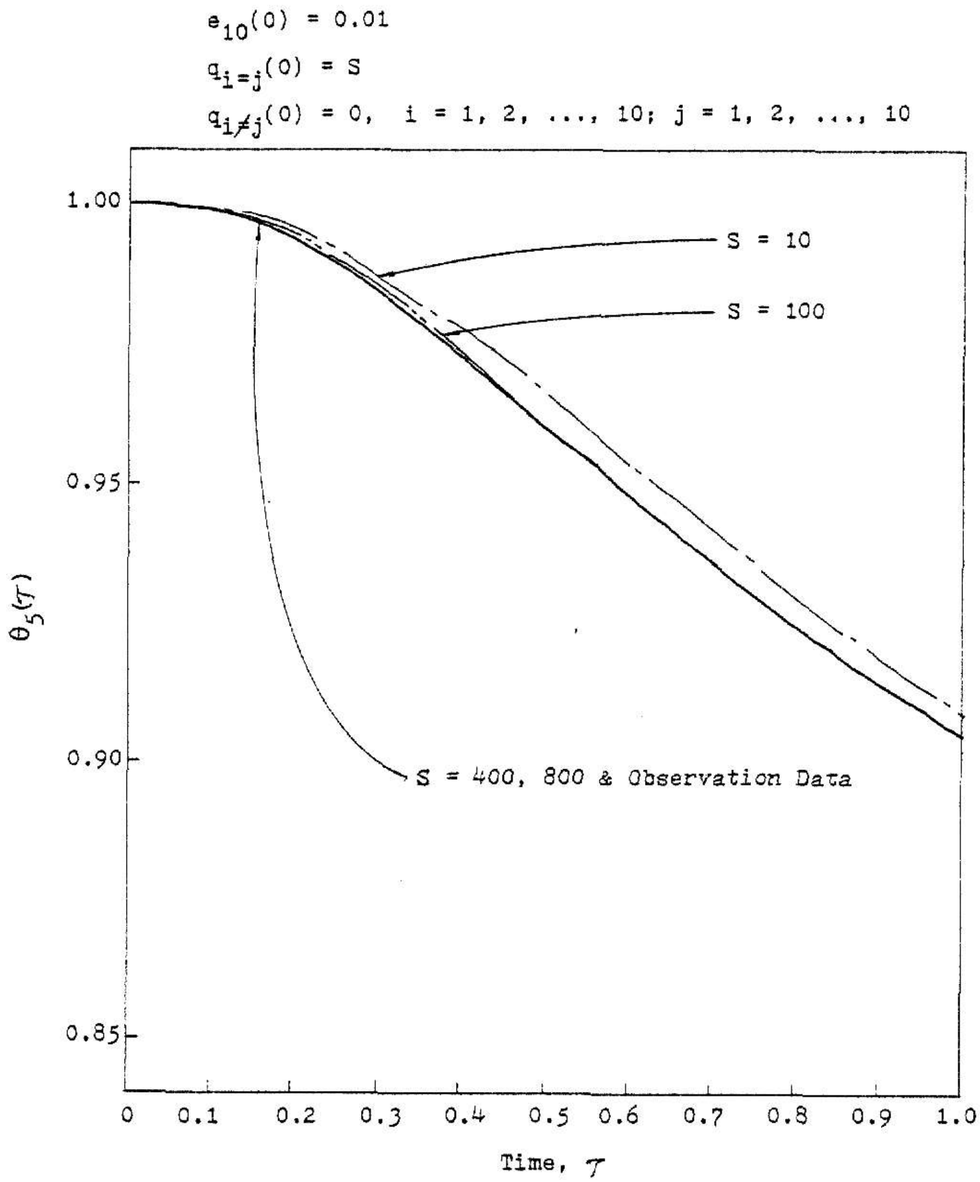

Figure 9. Estimated state $\theta_5(\tau)$ as a function of $q_{i=j}(0)$

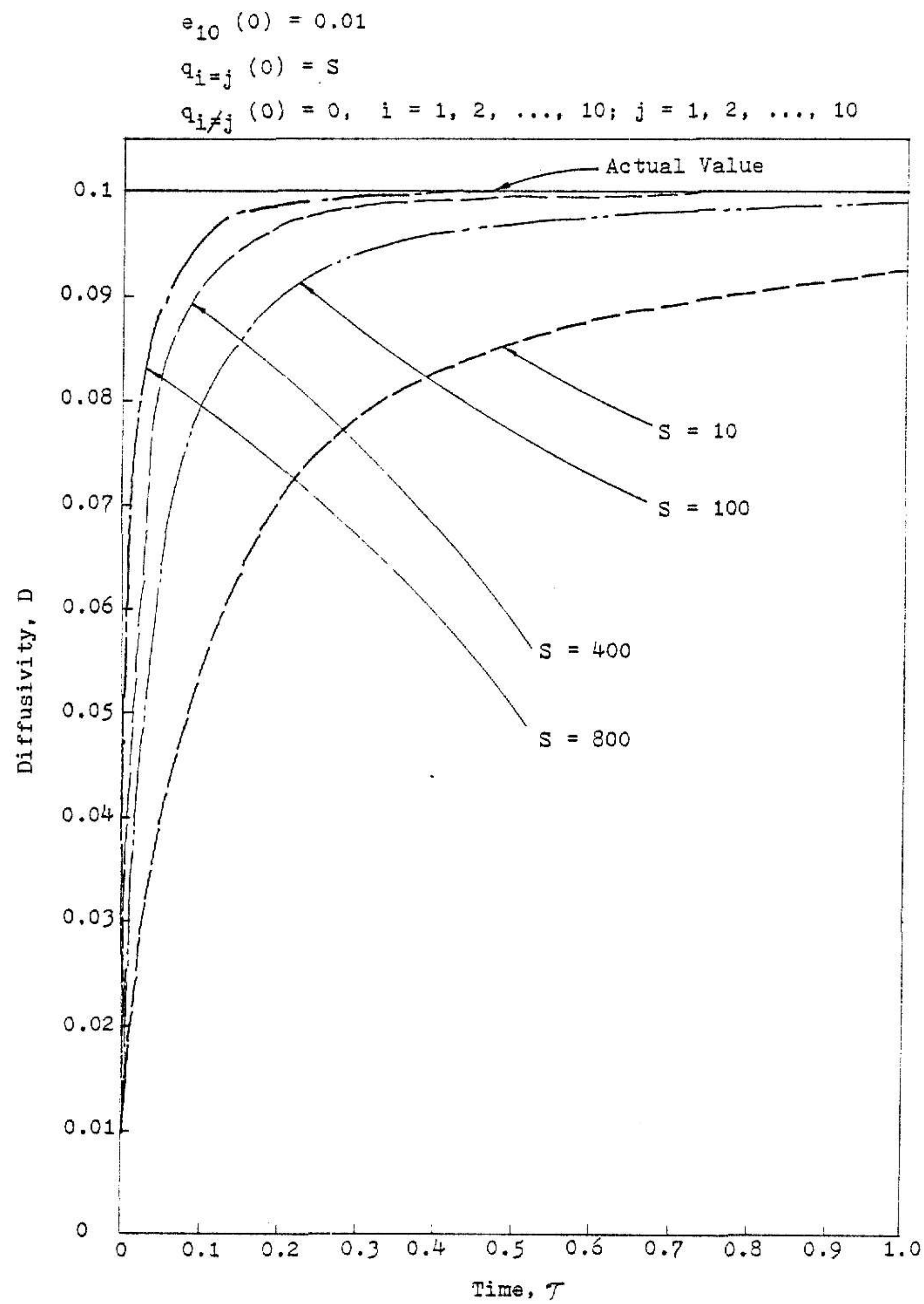

Figure 10. Estimated parameter D as a function of $q_{i=j}(0)$

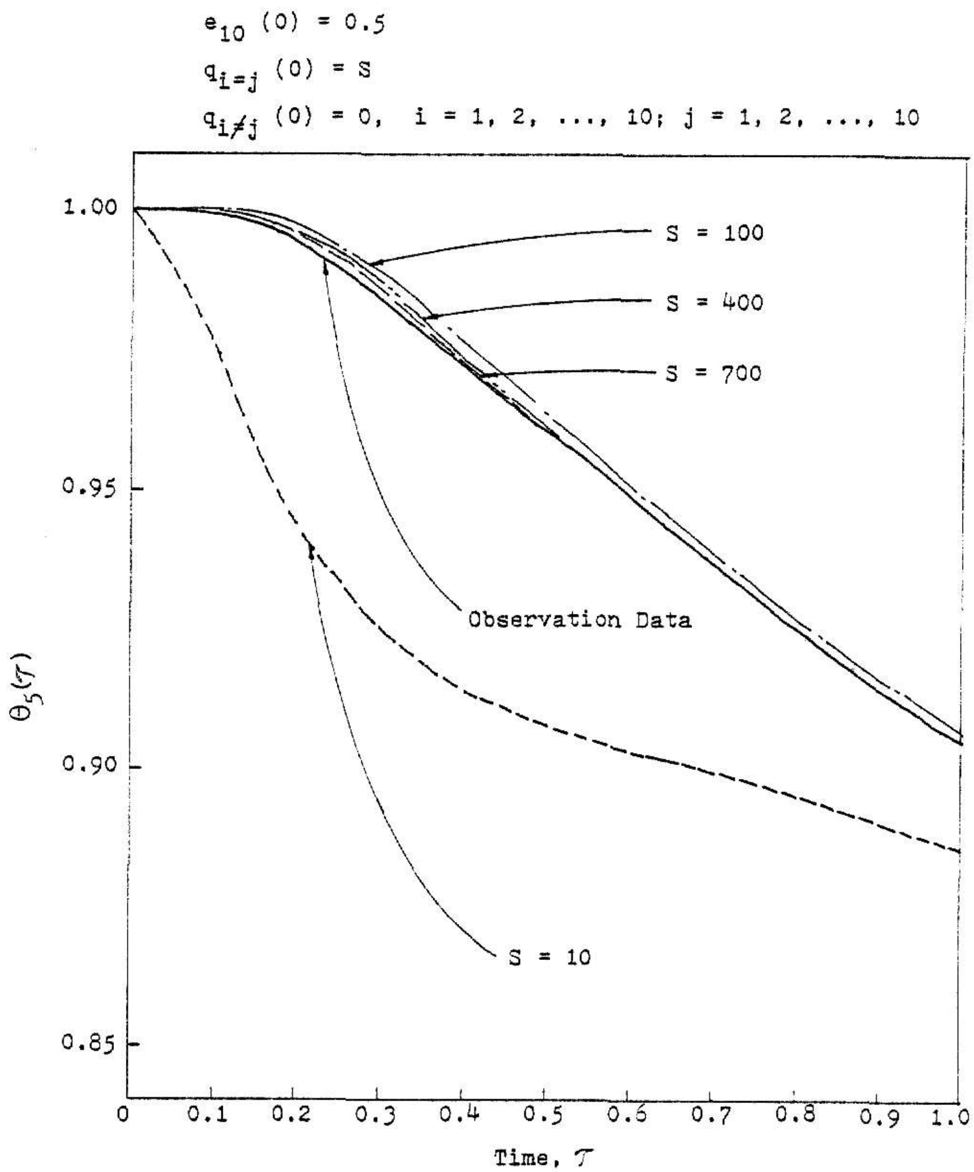

Figure 11. Estimated state $\theta_5(\tau)$ as a function of $q_{i=j}(0)$

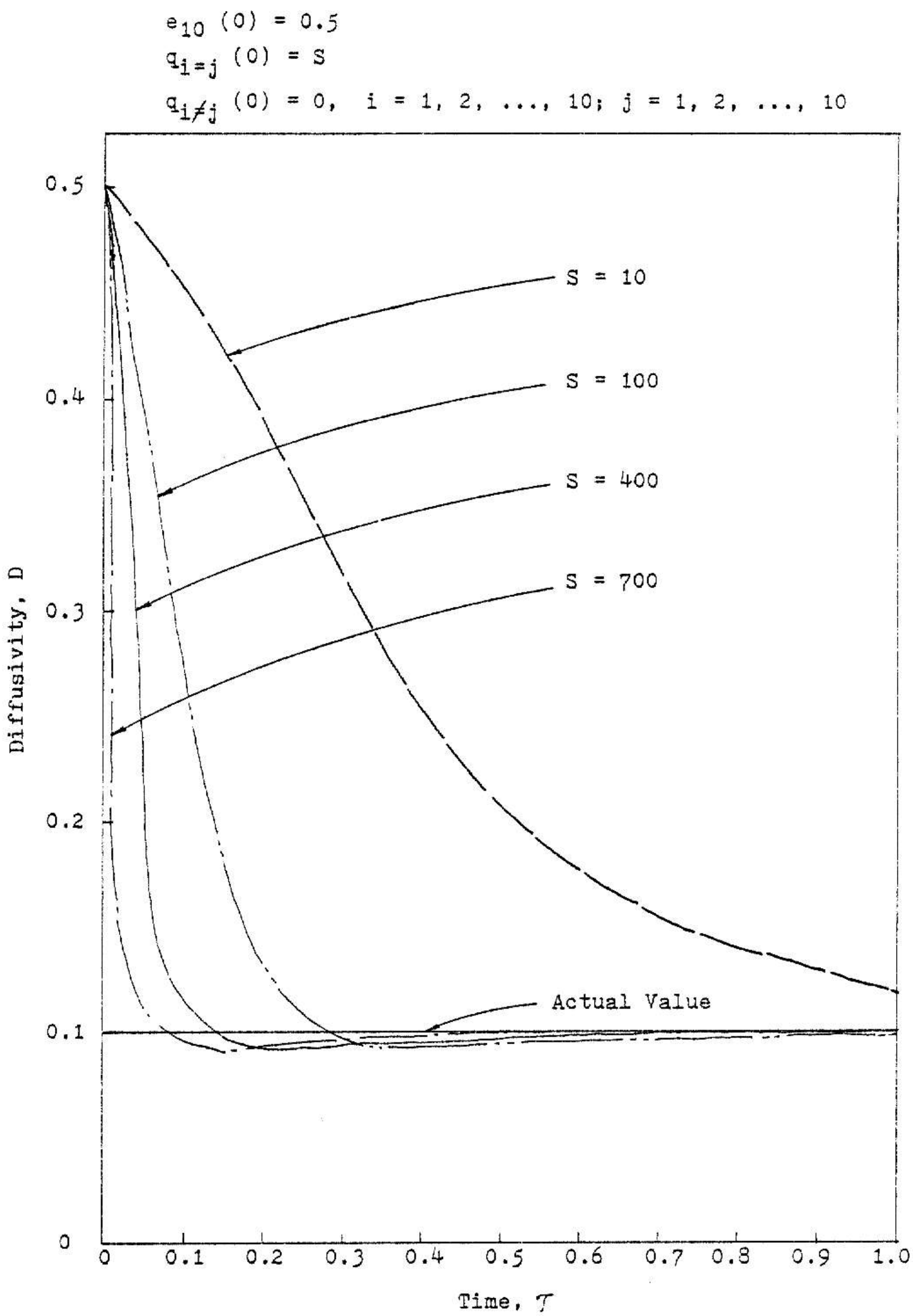

Figure 12. Estimated parameter D as a function of $q_{i=j}(0)$

where the other elements of Equations (4.18a) and (4.18b) remained the same. Figures 13 and 14 show the results of the estimated $\theta_5(\tau)$ and D, respectively. It is also shown that the convergence rates are improved with heavy weights on S. However, too heavy weights such as S = 700 made the solutions diverge.

4.5 DISCUSSION

The concept of invariant imbedding has been used to solve the estimation problem for both of state and parameter in an unconfined aquifer stream interaction system. Four numerical examples are solved. The latter three examples are related to finding the influence of the diagonal terms in the weighting function.

The numerical experiments seem to indicate the following. First, this approach appears to be an effective tool to estimate the state and the parameter in an unconfined aquifer stream interaction system as long as a proper weighting function is given. Second, the higher values of the diagonal terms of the weighting function give more accurate convergence values and faster convergence rates in this particular problem. However, too high values make the solutions diverge.

In this work, no noise on the observations has been assumed. Only the influence of the diagonal terms of the weighting function has been considered. It can also be one of the interesting problems to observe the effect of disturbances on the measurements and the effect of the non-diagonal terms of the

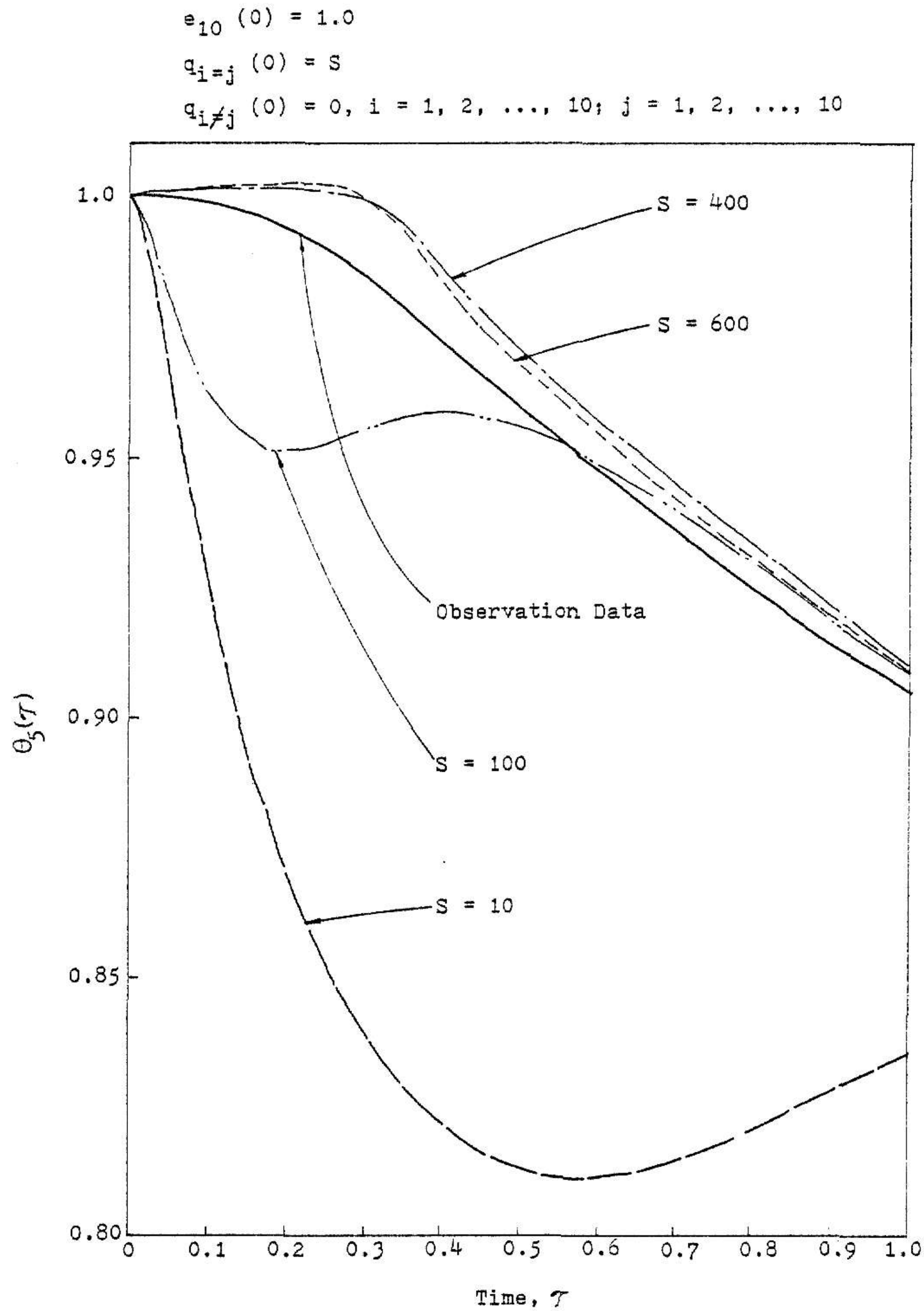

Figure 13. Estimated state $\theta_5(\tau)$ as a function of $q_{i=j}(0)$

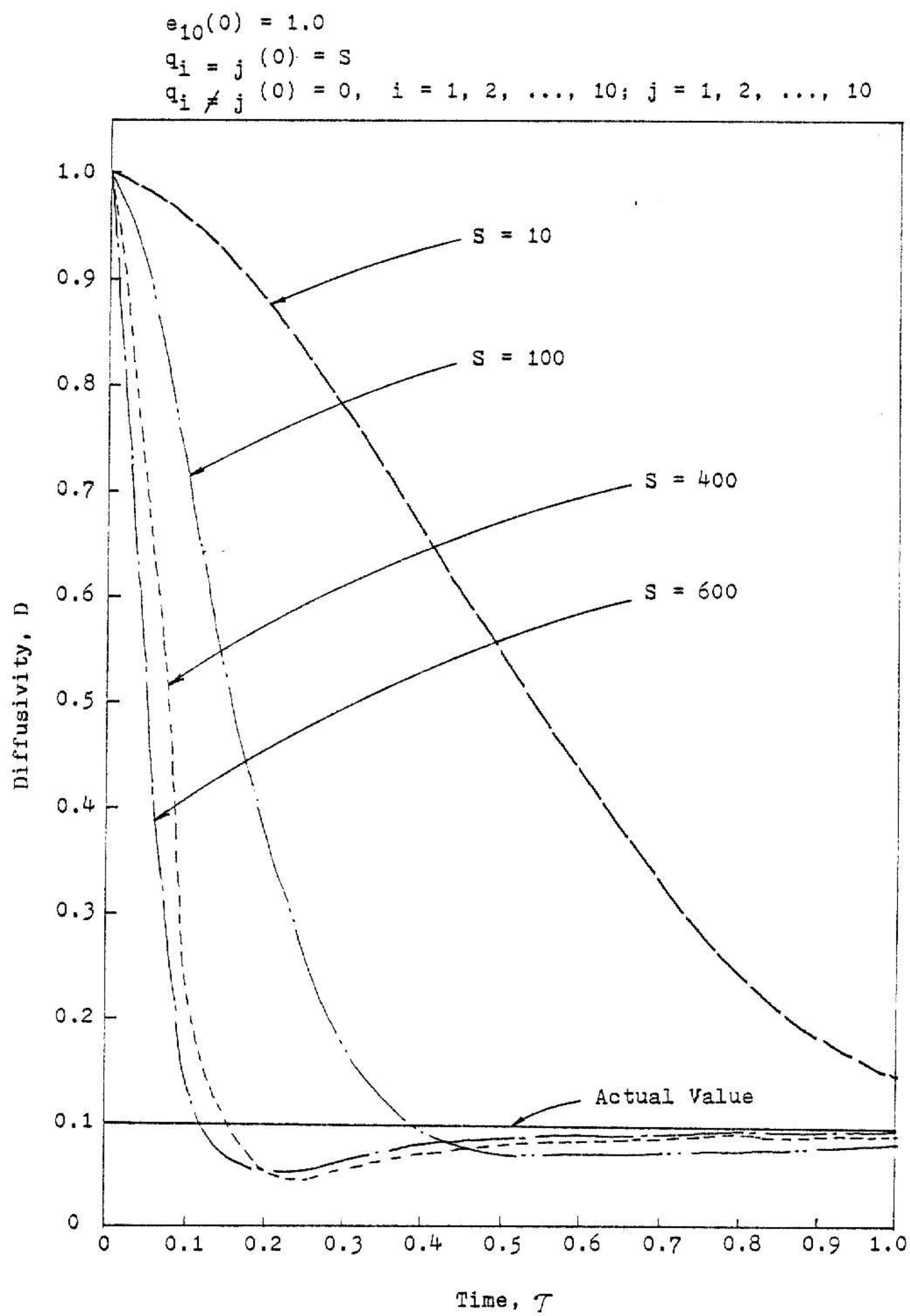

Figure 14. Estimated parameter D as a function of $q_{i=j}(0)$

weighting function. In order to find a more general rule related to the weighting function and investigate the effect of noise on the observation data, more computational work and research are needed.

CHAPTER 5

SUMMARY AND CONCLUSION

In an unconfined aquifer and stream interaction system, the governing equation is a second order nonlinear partial differential equation subject to the time varying boundary conditions for which no solution of closed form exists. The problem of interest is an inverse one; i.e., the observation data are given and the aquifer parameters imbedded in the governing equation are unknown. In this work, the observation data were generated using assumed values of parameters.

The technique of finite difference approximation has been used in order to replace the governing partial differential equation by a system of nonlinear ordinary differential equations. The quasilinearization technique and the concept of invariant imbedding have been applied to solve the aquifer parameter estimation problem. As has been shown in the numerical examples, the parameter estimation problems are effectively solved by two different approaches.

The most attractive property of the quasilinearization technique is its rapid convergence nature. Numerical results of the examples in this work indicate:

1. It converges very rapidly (within five iterations) to the correct answer even with very rough initial approximations.
2. High accuracy is obtained (five digit accuracy).
3. In general, it converges to the correct solution within

three to seven iterations as long as the initial approximations are within the interval of convergence.

No noises on the observation data have been assumed. In order to find the effect of noises on the estimation, more researches are needed.

Since the problem under consideration is essentially a two-point boundary value problem, it can also be solved by the invariant imbedding approach. By using invariant imbedding, the optimal sequential estimator equations have been obtained. These estimator equations, which are a system of ordinary differential equations of initial type, can be solved easily on computers. Numerical results indicate:

1. The estimated results are less accurate than those of quasilinearization. However, these results are still accurate enough for practical purpose.
2. The higher values of the diagonal terms of the weighting function give more accurate and faster convergence in this problem. However, too high values make the solutions diverge.

No disturbances on the observation data have been introduced. Only the influence of diagonal terms of the weighting function has been considered. It can be interesting to find the effect of noises on the observation data. It can also be one of the interesting problems to investigate the effect of non-diagonal terms of the weighting function. In order to find the effect of noises on the observation data and the effect of non-diagonal terms of the weighting function, more computational work and research are needed. The aquifer parameter has been considered as a pure constant. However, it is seen that the invariant imbedding approach can be extended to an estimation problem of aquifer parameter which is a function of space variable.

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APPENDICES

Computer Programs

APPENDIX 1.

COMPUTER PROGRAM FOR THE QUASILINEARIZATION ALGORITHM

```
C
C     ***************
C     * MAIN PROGRAM *
C     ***************
C
        IMPLICIT REAL*8(A-H,O-Z)
        DIMENSION Z(11,501),P(11,501),Q(11,501),T1(11,501),
       1          Y(10),DY(10),F(80)
      1 FORMAT(1H1)
      2 FORMAT(3I3,2D12.3)
      3 FORMAT(///,49X,29(1H*),/,  49X,1(1H*),27X,1(1H*),/,
       149X,1(1H*),' OBSERVATION DATA = Z(I,J) ',1(1H*),/,
       249X,1(1H*),27X,1(1H*),/,49X,29(1H*),///)
      4 FORMAT(1X,11D12.5)
      5 FORMAT(///)
      6 FORMAT(1X,' D = ',D12.5)
      7 FORMAT(1X,' SO = ',D12.5)
      8 FORMAT(//,39X,50(1H*),/,39X,50(1H*),/,39X,2(1H*),
       146X,2(1H*),/,39X,
       2'** OPTIMAL IDENTIFICATION OF AQUIFER PARAMETERS **',
       3/,39X,
       4'**          USING  QUASI-LINEARIZATION           **',
       5/,39X,2(1H*),46X,2(1H*),/,39X,50(1H*),/,39X,50(1H*))
       346X,2(1H*),/,39X,50(1H*),/,39X,50(1H*))
      9 FORMAT(3D12.3)
        WRITE(6,1)
        WRITE(6,8)
        READ(5,2) NPTS,N,IMAX,DELT,DIV
        READ(5,9) EPSI,DELY,DC
        D1=0.
C
C     ***************************
C     * DUMMY VALUES FOR T1(I,J) *
C     ***************************
C
        DO 713 I=1,NPTS
        DO 713 J=1,IMAX
        T1(I,J)=0.D0
    713 CONTINUE
C
C     ***********************************************************
C     * TO GET OBSERVATION DATA(Z(A)), INTEGRATE THE GOVERNING
C     * EQUATION SUBJECT TO INITIAL & BOUNDARY CONDITIONS *****
C     *******************************************************
C
        NA=1
        DO 702 I=1,N
        Y(I)=1.D0
    702 CONTINUE
        DO 703 KK=1,IMAX
        CALL  RKG(KK,DELT,N,Y,F,L,M,J,NA,DIV,D1,DELY,T1)
        DO 704 I=2,NPTS
        Z(I,KK)=Y(I-1)
    704 CONTINUE
        IF(KK.EQ.1) Z(1,KK)=1.D0
        IF(KK.NE.1) Z(1,KK)=0.5D0
    703 CONTINUE
C
C     ********************
C     * PRINT OUT Z(I,J) *
```

```
C     ********************
C
         WRITE(6,3)
         DO 700 I=1,IMAX,5C
         WRITE(6,4) (Z(J,I),J=1,NPTS)
   700   CONTINUE
C
C     *******************************************************
C     * INTEGRATE NON-LINEAR DIFFERENTIAL EQUATION USING DO *
C     *******************************************************
C
         NA=1
         DO 710 I=1,N
         Y(I)=1.DO
   710   CONTINUE
         DO 711 KK=1,IMAX
         CALL RKG(KK,DELT,N,Y,F,L,M,J,NA,DC,D1,DELY,T1)
         DO 712 I=2,NPTS
         T1(I,KK)=Y(I-1)
   712   CONTINUE
         IF(KK.EQ.1) T1(1,KK)=1.DO
         IF(KK.NE.1) T1(1,KK)=C.5DC
   711   CONTINUE
         WRITE(6,5)
         WRITE(6,6) DO
         WRITE(6,5)
         DO 720 I=1,IMAX,5C
         WRITE(6,4) (T1(J,I),J=1,NPTS)
   720   CONTINUE
         SSUM=0.
         DO 721 J=1,IMAX,5C
         SSUM=SSUM+(T1(6,J)-Z(6,J))**2
   721   CONTINUE
         WRITE(6,7) SSUM
         WRITE(6,5)
C
C     ***********************************************
C     * INTEGRATE PARTICULAR EQUATIONS TO GET NEW D1 *
C     ***********************************************
C
   111   CONTINUE
C
C     ****************************
C     * PARTICULAR EQUATION --- P *
C     ****************************
C
         NA=2
         DO 21 I=1,N
         Y(I)=0.DO
    21   CONTINUE
         DO 22 KK=1,IMAX
         CALL RKG(KK,DELT,N,Y,F,L,M,J,NA,DC,D1,DELY,T1)
         DO 23 I=2,NPTS
         P(I,KK)=Y(I-1)
    23   CONTINUE
         IF(KK.EQ.1) P(1,KK)=0.DO
         IF(KK.NE.1) P(1,KK)=0.5DO
    22   CONTINUE
C
C     ****************************
```

```
C    * PARTICULAR SOLUTICN --- Q *
C    ****************************
C
       NA=3
       DO 31 I=1,N
       Y(I)=1.0D0
    31 CONTINUE
       DO 32 KK=1,IMAX
       CALL RKG(KK,DELT,N,Y,F,L,M,J,NA,D0,D1,DELY,T1)
       DO 33 I=2,NPTS
       Q(I,KK)=Y(I-1)
    33 CONTINUE
       IF(KK.EQ.1) Q(1,KK)=1.D0
       IF(KK.NE.1) Q(1,KK)=0.5D0
    32 CONTINUE
C
C    ************************************************************
C    * FIND D1 AT THE 5TH DISCRETIZED POINT-ASSUME UNIFORM *
C    * WJ OF 1 ***********************************************
C    ************************************************************
C
       ASUM=0.
       BSUM=0.
       DO 41 J=1,IMAX
       ASUM=ASUM+(Z(6,J)*P(6,J)-Q(6,J)*P(6,J))
       BSUM=BSUM+(P(6,J)*P(6,J))
    41 CONTINUE
       D1=ASUM/BSUM
C
C    ********************************************************
C    * INTEGRATE THE GOVERNING EQUATION USING NEW D1 *
C    ********************************************************
C
       NA=1
       DO 80 I=1,N
       Y(I)=1.D0
    80 CONTINUE
       DO 82 KK=1,IMAX
       CALL RKG(KK,DELT,N,Y,F,L,M,J,NA,D1,D0,DELY,T1)
       DO 83 I=2,NPTS
       P(I,KK)=Y(I-1)
    83 CONTINUE
       IF(KK.EQ.1) P(1,KK)=1.D0
       IF(KK.NE.1) P(1,KK)=0.5D0
    82 CONTINUE
       WRITE(6,5)
       WRITE(6,6) D1
       WRITE(6,5)
       DO 85 I=1,IMAX,50
       WRITE(6,4) (P(J,I),J=1,NPTS)
    85 CONTINUE
C
C    ****************************
C    * LEAST SQUARES CRITERICN *
C    ****************************
C
       SSUM=0.
       DO 55 J=1,IMAX,50
       SSUM=SSUM+(P(6,J)- Z(6,J))**2
    55 CONTINUE
```

```
      WRITE(6,7) SSUM
      WRITE(6,5)
      IF(SSUM.LE.EPSI) GO TO 999
C
C   ******************************************************
C   * INTEGRATE THE LINEARIZED EQUATION USING D0, D1 & T1 *
C   * TO GET NEW T1 ***************************************
C   ******************************************************
C
      NA=4
      DO 53 I=1,N
      Y(I)=1.D0
   53 CONTINUE
      DO 71 KK=1,IMAX
      CALL RKG(KK,DELT,N,Y,F,L,M,J,NA,D0,D1,DELY,T1)
      DO 72 I=2,NPTS
      T1(I,KK)=Y(I-1)
   72 CONTINUE
      IF(KK.EQ.1) T1(1,KK)=1.D0
      IF(KK.NE.1) T1(1,KK)=0.5D0
   71 CONTINUE
      D0=D1
      GO TO 111
  999 CONTINUE
      WRITE(6,1)
      STOP
      END
```

```
C
C
      SUBROUTINE RKG(KK,DT,N,Y,F,L,M,J,NA,DC,D1,DELY,TA)
C
C
C    ***********************************
C    * RUNGE-KUTTA FOURTH ORDER METHOD *
C    ***********************************
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(10),DY(10),F(80),TA(11,501)
      T=(KK-1)*DT
      IF (KK.GT.1) GO TO 700
  310 L=3
      M=0
  700 CONTINUE
      GO TO (100,110,300),L
  100 GO TO (101,110),IG
  101 J = 1
      L = 2
      DO 106 K = 1,N
      K1 = K+3*N
      K2 = K1+N
      K3 = N + K
      F(K1) = Y(K)
      F(K3) = F(K1)
  106 F(K2) = DY(K)
      GO TO 406
  110 DO 140 K=1,N
      K1 = K
      K2 = K+5*N
      K3 = K2+N
      K4 = K + N
      GO TO (111,112,113,114),J
  111 F(K1) = DY(K)*DT
      Y(K) = F(K4)+.5*F(K1)
      GO TO 140
  112 F(K2) = DY(K)*DT
      GO TO 124
  113 F(K3) = DY(K)*DT
      GO TO 134
  114 Y(K) = F(K4) +(F(K1)+2.*(F(K2)+F(K3))+DY(K)*DT)/6.
      GO TO 140
  124 Y(K) = .5*F(K2)
      Y(K) = Y(K)+F(K4)
      GO TO 140
  134 Y(K) = F(K4)+F(K3)
  140 CONTINUE
      GO TO (170,180,170,180),J
  170 T = T + .5*DT
  180 J = J+1
      IF (J-4)404,404,299
  299 M=1
      GO TO 406
  300 IG =1
      GO TO 405
  404 IG=2
  405 L=1
  406 CONTINUE
      IF(M-1) 710,310,710
```

```
710 GO TO (500,999,999),L
500 CALL FCT(KK,Y,DY,NA,DO,D1,DELY,TA)
    GO TO 700
999 RETURN
    END
```

```
C
C
      SUBROUTINE FCT(JK,Y,DY,NUMBER,D0,D1,DELY,TA)
C
C
C    *******************************
C    * SELECTION OF PROPER EQUATION *
C    *******************************
C
      IMPLICIT REAL*8(A-H,C-Z)
      DIMENSION Y(10),DY(10),TA(11,501)
      J=JK
      DEL=2*DELY*DELY
      GO TO (10,20,30,40),NUMBER
   10 CONTINUE
C
C    *************************************
C    * THE GOVERNING (NON-LINEAR) EQUATION *
C    *************************************
C
      IF(J.EQ.1) GO TO 101
      DY(1)=D0*(Y(2)**2-2*Y(1)**2+(0.5D0)**2)/DEL
      GO TO 102
  101 CONTINUE
      DY(1)=D0*(Y(2)**2-2*Y(1)**2+1.0D0)/DEL
  102 CONTINUE
      DO 103 I=2,9
      DY(I)=D0*(Y(I+1)**2-2*Y(I)**2+Y(I-1)**2)/DEL
  103 CONTINUE
      DY(10)=DY(9)
      RETURN
   20 CONTINUE
C
C    ********************
C    * THE EQUATION FOR P *
C    ********************
C
      DY(1)=Y(1)*(D0*(-4*TA(2,J))/DEL)+Y(2)*(D0*(2*TA(3,J))
     1/DEL) +((   TA(3,J)**2-2*   TA(2,J)**2+   TA(1,J)**2)
     2/DEL)
      DO 201 I=2,9
      DY(I)=Y(I)*(D0*(-4*   TA(I+1,J))/DEL)+
     1      Y(I+1)*(D0*(2*   TA(I+2,J))/DEL)+
     2      Y(I-1)*(D0*(2*   TA(I,J))/DEL)+
     3     ((   TA(I+2,J)**2-2*TA(I+1,J)**2+TA(I,J)**2)/DEL)
  201 CONTINUE
      DY(10)=DY(9)
      RETURN
   30 CONTINUE
C
C    ********************
C    * THE EQUATION FOR C *
C    ********************
C
      DY(1)=(Y(1)-   TA(2,J))*(D0*(-4*   TA(2,J))/DEL)+
     1      (Y(2)-   TA(3,J))*(D0*(2*   TA(3,J))/DEL)
      DO 301 I=2,9
      DY(I)=(Y(I)-   TA(I+1,J))*(D0*(-4*   TA(I+1,J))/DEL)+
     1      (Y(I+1)-   TA(I+2,J))*(D0*(2*   TA(I+2,J))/DEL)
     2      +(Y(I-1)-   TA(I,J))*(D0*(2*   TA(I,J))/DEL)
```

```
  301 CONTINUE
      DY(10)=DY(9)
      RETURN
   40 CONTINUE
C
C     ************************************
C     * THE LINEARIZED EQUATICN FOR THETA *
C     ************************************
C
      DY(1)=D0*(    TA(3,J)**2-2*TA(2,J)**2+TA(1,J)**2)/DEL+
     1      (Y(1)-    TA(2,J))*(D0*(-4*    TA(2,J))/DEL)+
     2      (Y(2)-    TA(3,J))*(DC*(2*    TA(3,J))/DEL)+
     3      (D1-D0)*((TA(3,J)**2-2*TA(2,J)**2+TA(1,J)**2)/DEL)
      DO 401 I=2,9
      DY(I)=D0*(TA(I+2,J)**2-2*TA(I+1,J)**2+TA(I,J)**2)/DEL
     1      +(Y(I)-    TA(I+1,J))*(D0*(-4*    TA(I+1,J))/DEL)+
     2      (Y(I+1)-    TA(I+2,J))*(D0*(2*    TA(I+2,J))/DEL)+
     3      (Y(I-1)-    TA(I,J))*(D0*(2*    TA(I,J))/DEL)+
     4      (D1-D0)*((    TA(I+2,J)**2-2*    TA(I+1,J)**2+
     5     TA(I,J)**2)/DEL)
     5      DEL)
  401 CONTINUE
      DY(10)=DY(9)
      RETURN
      END
```

APPENDIX 2.

COMPUTER PROGRAM FOR THE INVARIANT IMBEDDING APPROACH

```
C
C     ****************
C     * MAIN PROGRAM *
C     ****************
C
      IMPLICIT REAL*8(A-H,C-Z)
      DIMENSION E(150),Z(11,501),H(11,11),HT(11,11),
     1          G(11,11),FT(1050)
    1 FORMAT(1H1)
    2 FORMAT(3I3,2D12.3)
    3 FORMAT(///,49X,29(1H*),/,  49X,1(1H*),27X,1(1H*),/,
     149X,1(1H*),
     2' OBSERVATION DATA = Z(I,J) ',1(1H*),/,49X,1(1H*),27X,
     31(1H*),/,49X,29(1H*),///)
    4 FORMAT(1X,11D12.5)
    5 FORMAT(//,44X,17(1H*),/,44X,1(1H*),15X,1(1H*),/,44X,
     1'* MATRIX H(E,A) *',/,
     244X,1(1H*),15X,1(1H*),/,44X,17(1H*),//)
    6 FORMAT(1X,11D10.2)
    7 FORMAT(//,40X,18(1H*),/,40X,1(1H*),16X,1(1H*),/,40X,
     1'* MATRIX H(E,A)T *',/,40X,1(1H*),16X,1(1H*),/,40X,
     218(1H*),//)
    8 FORMAT(//,39X,50(1H*),/,39X,50(1H*),/,39X,2(1H*),46X,
     12(1H*),/,39X,
     2'** OPTIMAL IDENTIFICATION OF AQUIFER PARAMETERS **',
     3/,39X,
     4'**             USING INVARIANT IMBEDDING            **',
     5/,39X,2(1H*),46X,2(1H*),/,39X,50(1H*),/,39X,50(1H*))
   11 FORMAT(I5,5X,7D10.3)
   12 FORMAT(///,130(1H*),//,1X,14(1H*),/,1X,1(1H*),12X,
     11(1H*),/,1X,
     2'* TRIAL DATA *',/,1X,1(1H*),12X,1(1H*),/,1X,14(1H*))
   13 FORMAT(//,5X,'E(1)=...=E(9)= ',D10.3,3X,'E(10)=D= ',
     1D10.3)
   14 FORMAT(///,5X,'TRIAL NO= ',I3,3X,'Q(I#J) = ',D10.3,3X,
     1'Q(I=J) = ',D10.3,//)
      WRITE(6,1)
      WRITE(6,8)
      READ(5,2) NPTS,N,IMAX,DELT,DIV
      NM1=N-1
      NN=N*N
      NODE=NN+N
      DELY=0.1D0
C
C     ***********************************************************
C     * TO GET OBSERVATION DATA(Z(A)), INTEGRATE THE GOVERNING
C     * EQUATION SUBJECT TO INITIAL & BOUNDARY CONDITIONS *****
C     *****************************************************
C
      CALL OBS(NPTS,IMAX,DELT,Z,DIV,DELY)
C
C     ********************
C     * PRINT OUT Z(I,J) *
C     ********************
C
      WRITE(6,3)
      DO 700 I=1,IMAX,50
      WRITE(6,4) (Z(J,I),J=1,NPTS)
  700 CONTINUE
C
```

```
C     ******************************************
C     * INPUT CATA OF H(E,A) ; (N-1)*N MATRIX *
C     ******************************************
C
      DO 701 I=1,NM1
      DO 701 J=1,NM1
      H(I,J)=0.
      IF(I.EQ.J) H(I,J)=1.
  701 CONTINUE
      DO 702 I=1,NM1
      H(I,N)=0.
  702 CONTINUE
C
C     ************************
C     * ECHO CHECK OF H(E,A) *
C     ************************
C
      WRITE(6,5)
      DO 703 I=1,NM1
      WRITE(6,6) (H(I,J),J=1,N)
  703 CONTINUE
C
C     **********************************
C     * CONSTRUCT HT = TRANSPOSE OF H *
C     **********************************
C
      CALL TRANSP(H,NM1,N,HT)
C
C     *************************
C     * ECHO CHECK OF H(E,A)T *
C     *************************
C
      WRITE(6,7)
      DO 710 I=1,N
      WRITE(6,6) (HT(I,J),J=1,NM1)
  710 CONTINUE
C
      WRITE(6,12)
C
C
C     ****************************************
C     * INITIALIZE E ;  E(N)=D---DIFFUSIVITY *
C     ****************************************
C
  666 CONTINUE
      READ(5,11) ITRLE,ENE,EEQ
      IF(ITRLE.EQ.999) GO TO 999
      WRITE(6,13) ENE,EEQ
  555 CONTINUE
      DO 705 I=1,N
      IF(I.NE.N) E(I)=ENE
      IF(I.EQ.N) E(I)=EEQ
  705 CONTINUE
C
C     ***************************
C     * INITIALIZE Q(A) =Q(I,J) *
C     ***************************
C
      READ(5,11) ITRLQ,QNE,QEQ
      IF(ITRLQ.EQ.99) GO TO 666
```

```
      WRITE(6,14) ITRLQ,QNE,QEQ
      DO 704 I=1,N
      DO 704 J=1,N
      Q(I,J)=QNE
      IF(I.EQ.J) Q(I,J)=QEQ
  704 CONTINUE
C
C    ******************************************************
C    * CONVERT Q(I,J) TO E(N+1),E(N+2), ...,E(NN-1),E(NN) *
C    ******************************************************
C
      KA=N+1
      DO 706 I=1,N
      DO 706 J=1,N
      E(KA)=Q(I,J)
      KA=KA+1
  706 CONTINUE
      T=0.
      IMAX=1.
      IRUN=1
      CALL OUTPUT(N,T,E)
C
C    **********************************************************
C    * INTEGRATE THE ESTIMATOR EQUATION USING THE RUNGE-KUTTA
C    * METHOD **************************************************
C    **********
C
  111 CONTINUE
      CALL RKT(IRUN,N,NODE,DELY,DELT,H,HT,Z,E,FT,LT,MT,JT)
      IF(IRUN.EQ.51) GO TO 222
      IF(IRUN.EQ.101) GO TO 222
      IF(IRUN.EQ.151) GO TO 222
      IF(IRUN.EQ.201) GO TO 222
      IF(IRUN.EQ.251) GO TO 222
      IF(IRUN.EQ.301) GO TO 222
      IF(IRUN.EQ.351) GO TO 222
      IF(IRUN.EQ.401) GO TO 222
      IF(IRUN.EQ.451) GO TO 222
      IF(IRUN.EQ.501) GO TO 222
      GO TO 333
  222 CONTINUE
      T=DFLOAT(IRUN-1)*DELT
      CALL OUTPUT(N,T,E)
  333 CONTINUE
      IRUN=IRUN+1
      IF(IRUN.GT.IMAX) GO TO 555
      GO TO 111
  999 CONTINUE
      WRITE(6,1)
      STOP
      END
```

```
C
C
      SUBROUTINE OBS(NPTS,IMAX,DELT,Z,DIV,DELY)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(10),DY(10),F(70),Z(11,501)
      N=NPTS-1
      DO 702 I=1,N
      Y(I)=1.D0
  702 CONTINUE
      DO 703 KK=1,IMAX
      CALL DRKG(KK,DELT,N,Y,F,L,M,J,DIV,DELY)
      DO 704 I=2,NPTS
      Z(I,KK)=Y(I-1)
  704 CONTINUE
      IF(KK.EQ.1) Z(1,KK)=1.D0
      IF(KK.NE.1) Z(1,KK)=0.5D0
  703 CONTINUE
      RETURN
      END
```

```
C
      SUBROUTINE DRKG(KK,DT,N,Y,F,L,M,J,DA,DL)
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(10),DY(10),F(70)
      T=(KK-1)*DT
      IF (KK.GT.1) GO TO 700
  310 L=3
      M=0
  700 CONTINUE
      GO TO (100,110,300),L
  100 GO TO (101,110),IG
  101 J=1
      L = 2
      DO 106 K = 1,N
      K1 = K+3*N
      K2 = K1+N
      K3 = N + K
      F(K1) = Y(K)
      F(K3) = F(K1)
  106 F(K2) = DY(K)
      GO TO 406
  110 DO 140 K=1,N
      K1 = K
      K2 = K+5*N
      K3 = K2+N
      K4 = K + N
      GO TO (111,112,113,114),J
  111 F(K1) = DY(K)*DT
      Y(K) = F(K4)+.5*F(K1)
      GO TO 140
  112 F(K2) = DY(K)*DT
      GO TO 124
  113 F(K3) = DY(K)*DT
      GO TO 134
  114 Y(K) = F(K4) +(F(K1)+2.*(F(K2)+F(K3))+DY(K)*DT)/6.
      GO TO 140
  124 Y(K) = .5*F(K2)
      Y(K) = Y(K)+F(K4)
      GO TO 140
  134 Y(K) = F(K4)+F(K3)
  140 CONTINUE
      GO TO (170,180,170,180),J
  170 T = T + .5*DT
  180 J = J+1
      IF (J-4)404,404,299
  299 M=1
      GO TO 406
  300 IG =1
      GO TO 405
  404 IG=2
  405 L=1
  406 CONTINUE
      IF(M-1) 710,310,710
  710 GO TO (500,999,999),L
  500 CALL FCTO(KK,Y,DY,DA,DL)
      GO TO 700
  999 RETURN
      END
```

```
C
C
      SUBROUTINE FCTO(JK,Y,DY,DIV,DELY)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(10),DY(10)
      DEL=1./(2.*DELY**2)
      IF(JK.EQ.1) GO TO 10
      DY(1)=  DEL*DIV*(Y(2)**2-2.*Y(1)**2+(0.5D0)**2)
      GO TO 20
   10 CONTINUE
      DY(1)=  DEL*DIV*(Y(2)**2-2.*Y(1)**2+1.0D0)
   20 CONTINUE
      DO 70  I=2,9
      DY(I)=  DEL*DIV*(Y(I+1)**2-2.*Y(I)**2+Y(I-1)**2)
   70 CONTINUE
      DY(10)=DY(9)
      RETURN
      END
```

```
C
      SUBROUTINE RKT(KK,NF,N,DELY,DT,H,HT,Z,Y,F,L,M,J)
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Y(150),DY(150),F(1050),H(11,11),HT(11,11),
     1          Z(11,501)
      T=(KK-1)*DT
      IF (KK.GT.1) GO TO 700
  310 L=3
      M=0
  700 CONTINUE
      GO TO (100,110,300),L
  100 GO TO (101,110),IG
  101 J=1
      L = 2
      DO 106 K = 1,N
      K1 = K+3*N
      K2 = K1+N
      K3 = N + K
      F(K1) = Y(K)
      F(K3) = F(K1)
  106 F(K2) = DY(K)
      GO TO 406
  110 DO 140 K=1,N
      K1 = K
      K2 = K+5*N
      K3 = K2+N
      K4 = K + N
      GO TO (111,112,113,114),J
  111 F(K1) = DY(K)*DT
      Y(K) = F(K4)+.5*F(K1)
      GO TO 140
  112 F(K2) = DY(K)*DT
      GO TO 124
  113 F(K3) = DY(K)*DT
      GO TO 134
  114 Y(K) = F(K4) +(F(K1)+2.*(F(K2)+F(K3))+DY(K)*DT)/6.
      GO TO 140
  124 Y(K) = .5*F(K2)
      Y(K) = Y(K)+F(K4)
      GO TO 140
  134 Y(K) = F(K4)+F(K3)
  140 CONTINUE
      GO TO (170,180,170,180),J
  170 T = T + .5*DT
  180 J = J+1
      IF (J-4)404,404,299
  299 M=1
      GO TO 406
  300 IG =1
      GO TO 405
  404 IG=2
  405 L=1
  406 CONTINUE
      IF(M-1) 710,310,710
  710 GO TO (500,999,999),L
  500 CALL FCT(KK,NF,N,DELY,DT,H,HT,Y,DY,Z)
      GO TO 700
  999 RETURN
      END
```

```
C
C
      SUBROUTINE FCT(KTIME,N,NODE,DY,DT,HEA,HEAT,E,F,Z)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION FEA(11),E(150),ZE(11),Z(11,501),HEA(11,11),
     1          Q(11,11),C(11,11),COE(11,1),EA(11,1),F(150),
     2          FEAQ(11,11),QFET(11,11),FEEAT(11,11),
     3          FEEA(11,11),C1(11,11),C2(11,11),C3(11,11),
     4          HEAT(11,11),S1(11,11),S2(11,11)
      NM1=N-1
      DEL=E(N)/(2.*DY**2)
C
C    ***************************
C    * CONSTRUCT MATRIX F(E,A) *
C    ***************************
C
      DO 700 I=1,N
      IF(I.EQ.1.AND.KTIME.EQ.1) GO TO 800
      IF(I.EQ.1.AND.KTIME.NE.1) GO TO 801
      IF(I.EQ.NM1) GO TO 802
      IF(I.EQ.N) GO TO 803
      FEA(I)=DEL*(E(I+1)**2-2.*E(I)**2+E(I-1)**2)
      GO TO 700
  800 CONTINUE
      FEA(I)=DEL*(E(I+1)**2-2.*E(I)**2+1.0D0)
      GO TO 700
  801 CONTINUE
      FEA(I)=DEL*(E(I+1)**2-2.*E(I)**2+0.5**2)
      GO TO 700
  802 CONTINUE
      FEA(I)=DEL*(-E(I)**2+E(I-1)**2)
      GO TO 700
  803 CONTINUE
      FEA(I)=0.D0
  700 CONTINUE
C
C    ************************
C    * MATRIX (Z(A)-H(E,A)) *
C    ************************
C
      DO 701 I=1,NM1
      ZE(I)=Z(I+1,KTIME)-E(I)
  701 CONTINUE
C
C    ***************
C    * MATRIX Q(A) *
C    ***************
C
      KQ=N+1
      DO 702 I=1,N
      DO 702 J=1,N
      Q(I,J)=E(KQ)
      KQ=KQ+1
  702 CONTINUE
C
C    ***********************************************
C    * EVALUATE DE/DA=F(E,A)+Q(A)*HE(E,A)T*(Z(A)-H(E,A)) *
C    ***********************************************
```

```
C
C
C     (1)  MULTIPLY Q(A)*(HE(E,A)T)
C
       CALL MATMPY(Q,N,N,HEAT,NM1,C)
C
C     (2)  MULTIPLY (1)*(Z(A)-H(E,A))
C
       CALL MATMPY(C,N,NM1,ZE,1,CCE)
C
C     (3)  ADD F(E,A)+(2)
C
       CALL MATADS(FEA,N,1,CCE,1,EA)
       DO 703 I=1,N
       F(I)=EA(I,1)
  703 CONTINUE
C
C    ***********************************************************
C    * EVALUATE DQ/DA=FE(E,A)*Q(A)+Q(A)*(FE(E,A)T)-Q(A)*(HE(
C    * E,A)T)*HE(E,A)*Q(A) ************************************
C
C
C     (1)  MATRIX FE(E,A)
C
       DO 704 I=1,N
       DO 704 J=1,N
       FEEA(I,J)=0.
  704 CONTINUE
       DO 705 I=1,NM1
       IF(I.EQ.1) GO TO 600
       IF(I.EQ.NM1) GO TO 500
       FEEA(I,I)=-4.*E(I)*DEL
       FEEA(I,I-1)=2.*E(I-1)*DEL
       FEEA(I,I+1)=2.*E(I+1)*DEL
       GO TO 705
  600 CONTINUE
       FEEA(I,I)=-4.*E(I)*DEL
       FEEA(I,I+1)=2.*E(I+1)*DEL
       GO TO 705
  500 CONTINUE
       FEEA(I,I)=-2.*E(I)*DEL
       FEEA(I,I-1)=2.*E(I-1)*DEL
  705 CONTINUE
       DO 706 I=1,N
       FEEA(I,N)=FEA(I)/E(N)
  706 CONTINUE
C
C     (2)  MULTIPLY FE(E,A)*Q(A)
C
       CALL MATMPY(FEEA,N,N,Q,N,FEAQ)
C
C     (3)  TRANSPOSE FE(E,A)
C
       CALL TRANSP(FEEA,N,N,FEEAT)
C
C     (4)  MULTIPLY Q(A)*(3)
C
       CALL MATMPY(Q,N,N,FEEAT,N,QFET)
C
C     (6)  CONSTRUCT Q(A)*HE(E,A)T
```

```
C
       CALL MATMPY(Q,N,N,HEAT,NM1,C1)
C
C     (7)  MULTIPLY (6)*HE(E,A)
C
       CALL MATMPY(C1,N,NM1,HEA,N,C2)
C
C     (8)  MULTIPLY (7)*G(A)
C
       CALL MATMPY(C2,N,N,G,N,C3)
C
C     (9)  ADD (2)+(4)
C
       CALL MATADS(FEAQ,N,N,GFET,1,S1)
C
C     (10)  SUBTRACT (9)-(8)
C
       CALL MATADS(S1,N,N,C3,2,S2)
       KQ=N+1
       DO 707 I=1,N
       DO 707 J=1,N
       F(KQ)=S2(I,J)
       KQ=KQ+1
  707 CONTINUE
       RETURN
       END
```

```
C
C
      SUBROUTINE TRANSP(A,N,M,B)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(11,11),B(11,11)
      DO 10 I=1,N
      DO 10 J=1,M
      B(J,I)=A(I,J)
   10 CONTINUE
      RETURN
      END
```

```
C
C
      SUBROUTINE MATMPY(A,N,M,B,L,C)
C
      IMPLICIT REAL*8(A-H,C-Z)
      DIMENSION A(11,11),B(11,11),C(11,11)
      DO 5 I=1,N
      DO 5 J=1,L
      C(I,J)=0.
      DO 5 K=1,M
      C(I,J)=C(I,J)+A(I,K)*B(K,J)
    5 CONTINUE
      RETURN
      END
```

```
C
C
      SUBROUTINE MATADS(A,N,M,B,L,C)
C
C
      IMPLICIT REAL*8(A-H,C-Z)
      DIMENSION A(11,11),B(11,11),C(11,11)
      GO TO (10,20),L
   10 CONTINUE
      DO 30 I=1,N
      DO 30 J=1,M
      C(I,J)=A(I,J)+B(I,J)
   30 CONTINUE
      RETURN
   20 CONTINUE
      DO 40 I=1,N
      DO 40 J=1,M
      C(I,J)=A(I,J)-B(I,J)
   40 CONTINUE
      RETURN
      END
```

```
C
C
      SUBROUTINE OUTPUT(N,T,E)
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION E(150),Q(11,11)
   10 FORMAT(2X,D12.5,2X,'*',2X,11D10.3)
   50 FORMAT(///)
   51 FORMAT(2X,23(1H*),/,2X,1(1H*),' TIME = ',F12.5,1X,
     111(1H*),/,2X,23(1H*),/)
   52 FORMAT(7X,'E(I)',50X,'Q(I,J)',//)
      KK=N+1
      DO 200 I=1,N
      DO 200 J=1,N
      Q(I,J)=E(KK)
      KK=KK+1
  200 CONTINUE
      WRITE(6,50)
      WRITE(6,51) T
      WRITE(6,52)
      DO 210 I=1,N
      WRITE(6,10) E(I),(Q(I,J),J=1,N)
  210 CONTINUE
      RETURN
      END
```

AQUIFER PARAMETER ESTIMATION BY QUASILINEARIZATION AND INVARIANT IMBEDDING

by

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Estimation of states and parameters in a mathematical model used in analyzing the system behaviour, is a frequent problem encountered in engineering, science and industries. Once a conceptual model is validated through experimental data, the model could be used to implement effective system control strategies.

Systematic procedures are presented to solve the estimation problem of aquifer diffusivity in an unconfined aquifer and stream interaction system. The fluctuation of the aquifer head is used as observations. The governing nonlinear partial differential equation is replaced by a system of nonlinear ordinary differential equations for which the technique of quasilinearization and the concept of invariant imbedding are applied.

The technique of quasilinearization is used to estimate the aquifer diffusivity. Numerical experiments are presented and compared with the published numerical results. The least squares criterion is used for the objective function. It is shown that only three to four iterations are needed to obtain five digit accuracy with very approximate initial guesses for the unknown parameter. The procedure is straightforward and converges quadratically.

The invariant imbedding approach is also used to estimate the aquifer heads and the diffusivity. In this approach, a sequential estimation scheme is obtained. By use of this sequential scheme, only current data are needed to estimate the current or future values of states and parameters. The classical least squares criterion is used to obtain the optimal estimates. It is seen that this approach appears to be an effective tool as long as a proper weighting function is given. The higher values of the diagonal terms of weighting function give more accurate convergence values and faster convergence rates. However, too high values make the solutions diverge.