

ESTIMATION OF PARAMETERS IN PARTIAL DIFFERENTIAL EQUATIONS--
WITH APPLICATIONS TO PETROLEUM RESERVOIR DESCRIPTION

Thesis by
Wen Hsiung Chen

In Partial Fulfillment of the Requirements
for the Degree of
Doctor of Philosophy

California Institute of Technology
Pasadena, California

1974

(Submitted November 19, 1973)

This thesis is dedicated to my parents.

ACKNOWLEDGMENT

I wish to express my sincere appreciation to my research advisor, Professor John H. Seinfeld, who provided encouragement and help and guided me with tireless patience throughout the course of this work.

Financial support from the California Institute of Technology in the form of Teaching and Research Assistantships, from the National Science Foundation, from the Chevron Oil Field Research Company and the Earle C. Anthony Foundation is gratefully acknowledged.

Finally, while I can acknowledge the years of patient understanding, encouragement, and financial support provided by my parents, I will never be able to thank them adequately. This thesis is a tribute to my parents.

ABSTRACT

The determination of parameters in dynamical systems, on the basis of noisy experimental data, is called the parameter estimation problem or inverse problem. In this dissertation, several methods for parameter estimation are derived for systems governed by partial differential equations, so-called distributed parameter systems.

The first class of problems, investigated in Chapter II, is that in which the parameters to be estimated are constants. This class of problems is important for it includes most cases of practical interest. Techniques based on gradient optimization, quasilinearization, and collocation methods are developed. A method of determining confidence intervals for parameter estimates is presented, a method which enables one to design experiments (and measurements) that lead to the best estimates of the parameters. The effectiveness of these methods for estimating constant parameters is illustrated through the estimation of the diffusivity in the heat equation, the estimation of the activation energy for a single reaction from dynamic plug flow reactor data, and the estimation of the permeabilities in a two-region reservoir model. The numerical results also show the advantage of using data taken at optimally chosen measurement locations to estimate the parameters.

Many physical systems contain spatially varying parameters, for example, the permeability distribution in a petroleum reservoir model. In Chapter III, two approaches are presented for the estimation of spatially varying parameters. The first is a method of steepest descent

based on consideration of the unknown parameter vector as a control vector. The second is based on treating the parameter as an additional state vector and employing least square filtering. The key feature of the former method is that the parameters are considered as continuous functions of position rather than as constant in a certain number of spatial regions. This technique may offer significant savings in computing time over conventional gradient optimization methods, such as steepest descent and Gauss-Newton in which the parameters are considered as uniform in a certain number of zones. Two examples are presented to illustrate the use of the method and its comparison to other algorithms.

In certain cases, the location of the boundary of a system may not be known, such as the boundary of a petroleum reservoir. In the case of oil reservoirs it is very important to be able to estimate the area and shape (or the location of the boundary) of a reservoir so that the production policies can be optimized. A method based on the variation of a functional defined on a variable region is developed in Chapter IV. The computational applications of this method are illustrated in determining the locations of the boundaries of a one-dimensional and a two-dimensional petroleum reservoir.

TABLE OF CONTENTS

ABSTRACT	
I. INTRODUCTION	1
II. ESTIMATION OF CONSTANT PARAMETERS IN PARTIAL DIFFERENTIAL EQUATIONS	
1. Introduction	5
2. Statement of the Problem	9
3. Computational Methods	11
3.1 Gradient Optimization Methods	12
3.2 Quasilinearization	16
3.3 Parameter Estimation Using Collocation	18
4. Accuracy of Constant Parameters Estimated in Partial Differential Equations	21
4.1 Theory	22
4.2 Applications	26
5. Examples	31
5.1 Example 1: Estimation of the Diffusivity in the Heat Equation	31
5.2 Example 2: Estimation of the Activation Energy for a Single Reaction	41
5.3 Example 3: Estimation of Petroleum Reservoir Permeabilities	46
5.4 Conclusions	49
Appendix II-A	53
Appendix II-B	56
Appendix II-C	64

III.	ESTIMATION OF SPATIALLY VARYING PARAMETERS IN PARTIAL DIFFERENTIAL EQUATIONS	
1.	Introduction	72
2.	General Formulation of the Problem	73
	Appendix III-A	76
	Appendix III-B	85
	Appendix III-C	100
IV.	ESTIMATION OF THE LOCATION OF THE BOUNDARY OF A DISTRIBUTED REGION--WITH APPLICATION TO PETROLEUM RESERVOIRS	
1.	Introduction	105
2.	Formulation of the Optimum Boundary Problem	106
3.	The Derivation of the Solution of the Optimum Boundary Problem	110
4.	Examples	
4.1	Example 1: Estimation of the Location of the Boundary for a One-Dimensional, One-Phase, Bounded Reservoir	124
4.2	Example 2: Estimation of the Location of the Boundary for a Two-Dimensional, One-Phase Reservoir with Constant Pressure Outer Boundary	127
5.	Conclusions	131
V.	CONCLUSIONS	140
	References	143
	Propositions	150

Chapter I

INTRODUCTION

A wide variety of physical problems of interest in physics, chemistry, and engineering are described by partial differential equations. In general, the form of the partial differential equations can be constructed from the laws of conservation of energy and of continuity of material up to a set of unknown parameters, which may be constants or functions of position, time, or both. Usually, these parameters can not be measured directly and, in fact, must be determined by minimizing some measure of the difference between noisy experimental measurements of the process and the solutions of the partial differential equations describing the process. This is commonly referred to as a parameter estimation, identification, or inverse problem. In this dissertation an attempt has been made to derive methods for determining both constant parameters and spatially varying parameters appearing in partial differential equations and associated boundary conditions.

In Chapter II three methods are presented for the estimation of constant parameters in distributed parameter systems. This class of parameters is important for it encompasses most cases of practical interest. First, because of the popularity and efficiency of steepest descent and quasilinearization in the estimation of constant parameters in ordinary differential equations, these methods are extended to the distributed parameter case. From a practical point of view, the amount of computing time required to solve the system model and sensitivity equations plays an important role because this is the most time

consuming part of the parameter estimation for distributed systems. With this in mind, a method based on collocation methods is derived. Three examples are used to illustrate the performance of these three methods. The comparison of the performance between the method of steepest descent and quasilinearization is then attempted.

Obviously, the values of parameters estimated from noisy data are of little value unless they are accompanied by an estimate of their reliability or accuracy. Although the measurements of a distributed system can, in principle, be placed anywhere within the domain of interest, it is necessary to make observations at a limited number of locations because of difficulty, significant expenditure for a complicated system, and the physical inaccessibility in obtaining the data. This means that we are required to extract as much information as possible from a small number of sensor locations. The question then arises--where and when should a fixed number of measurements be taken, which lead to the best estimates of parameters? Also, it is appropriate to ask what improvement in the accuracy of the estimates can be made with additional data? From the answer to this question one can justify whether the accuracy increase is worth the investment and effort, and hence whether the additional runs are profitable. These questions are also treated in Chapter II.

The estimation of constant parameters in differential equations has been studied extensively. However, relatively little has appeared in the literature concerning the estimation of spatially varying parameters in distributed parameter systems. In the past, spatially varying parameters have usually been assumed to be constant in a number

of zones which cover the whole spatial domain. Then the problem becomes the estimation of constant parameters. In Chapter III a new method, based on an optimal control formulation of the parameter estimation problem is developed. This method not only realistically treats the parameter as a continuous function of position, but also offers significant savings in the computational effort over the conventional "constant zone" methods. It should be noted that the extension of this approach to estimate time-varying or spatially varying and time-varying parameters in distributed parameter systems is straightforward. Two examples are used to examine the feasibility of this technique. In contrast to the optimal control formulation, the parameters can be considered as additional state variables, changing the problem into one of state estimation. This is also discussed in Chapter III.

In the above discussions we have assumed implicitly that the boundary of a distributed parameter system is fixed and the location of the boundary is specified. However, in some cases the boundary conditions of the system may be given, but the location of the boundary is not known. In order to completely define the physical model, the location of the boundary must be determined. A method for estimating the location of the boundary of a distributed system is derived in Chapter IV. From an economic point of view, to be attractive for this purpose a method should be able to determine the location of the boundary using observations which are made over a short period. We present two examples to demonstrate the estimation of the boundaries

of petroleum reservoirs utilizing data in the so-called late transient period, rather than requiring measurements in the pseudo-steady-state period.

Chapter II

ESTIMATION OF CONSTANT PARAMETERS IN PARTIAL DIFFERENTIAL EQUATIONS

1. Introduction

An important problem in process analysis is the estimation of parameters in a mathematical model from experimental data. Many systems of practical importance are described by partial differential equations containing unknown parameters which cannot be measured directly but which must be estimated on the basis of experimental data from the system--experimental data which will, in general, be corrupted by noise and errors.

Two basic parameter estimation schemes exist: non-sequential and sequential. In the former the estimation is carried out after all the data have been obtained, while in the latter the estimation is carried out continuously as the data are received. We will concentrate on non-sequential estimation since it represents the more common situation and since it is easier to implement in practice.

Several studies have appeared on the estimation of parameters in partial differential equations. Collins and Khatri [29] have proposed that finite differences be used to approximate the derivatives of state variables, and then the unknown parameters, which must appear linearly in the partial differential equations, are expressed as functions of the state variables at the mesh points. Although the method is conceptually simple, it is very sensitive to the level of measurement error and not generally useful. Beck [6-11] used a finite-difference method to solve the partial differential equation and then employed a least-squares method to determine the physical properties in the heat conduction

equation. This method is shown to be very effective when data with small errors are available and the initial estimates of parameters are close to the true values (say 10% in error). The modulating function method, originated by Shinbrot [71] and utilized by Loeb and Cahen [54] for determining the parameters of certain lumped systems, has been extended by Perdreauxville and Goodson [63] to determine the parameters of certain distributed parameter systems. The idea of this method is that the derivatives are reduced to those corresponding to the available data by operating on the partial differential equations with a function of known form (usually powers of sines) and integrating by parts. The result of the operation is a set of algebraic equations in the parameters. However, the partial differential equations may contain terms which cannot be treated by the method, and noise in the data affects the results significantly. Two extensions have been made based on the modulating function method. One was by Fairman and Shen [35] who discretized the derivatives in space to avoid the spatial integration and chose a modified form of the Poisson probability density function as the modulating function. The other one was by Tzafestas [74] who discretized the system in time and chose special modulating functions. It is well known that some classes of partial differential equations can be converted to a set of ordinary differential equations using the method of characteristics. Carpenter et al. [26] used this approach and a recursive stochastic gradient scheme to estimate the parameters in the resulting ordinary differential equations. Luckinbill and Childs [55] employed quasilinearization to estimate

parameters in partial differential equations from exact measurements. A combination of the method of characteristics and quasilinearization has been used to determine parameters in hyperbolic systems by Malpani and Donnelly [56]. Angel [2] presented a method combining Newton's method and discrete imbedding to estimate parameters in elliptic equations.

Methods based on the analytical solutions of partial differential equations have been proposed by Jones [48], Burggraf [18], Cannon et al. [19-24], Anderssen and White [1], Williams et al. [76], Clements [28], and Bellman et al. [12].

Recently, Polis et al. [64] have proposed an interesting method based on Galerkin's method which is similar to the collocation method proposed by Seinfeld and Chen [70]. The basic approach is to reduce the partial differential equations to a set of ordinary differential equations containing the parameters and then estimate unknown parameters by optimization schemes such as the method of steepest descent, search techniques and nonlinear filtering.

A general nonlinear least-squares filter for distributed systems has recently been derived by Huang, et al. [46] and Seinfeld, et al. [69]. Sequential parameter estimates can be generated by the filter from discrete noisy measurements. However, computationally this requires the solution of several partial differential equations, representing the estimator and covariance equations, and is not efficient for non-sequential analysis of experimental data.

The process of estimating parameters in models is not complete without an analysis of the accuracy of these parameters. So far the

literature available in this field deals only with the accuracy of parameter estimates in ordinary differential equations from discrete measurements. The method developed by Rosenbrock and Storey [66] is extended to parameter estimates in partial differential equations in this thesis.

One related important application of the analysis of the accuracy is to obtain the optimal location of the measurement points in a distributed parameter process such that the parameters can be determined as accurately as possible. This problem has been treated by Beck [7-11] and Badavas and Saridis [4]. Beck found the optimal measurement location by choosing the point where the sensitivity coefficient is maximum. The latter investigators employed a random optimization algorithm [59] to determine the location of the finite measurement point in a distributed region such that a sensitivity criterion is maximized. In Badavas and Saridis' paper, a positive definite matrix is obtained from the performance criterion in terms of the preselected approximating functions and the measurement points. The minimum eigenvalue of this matrix, which is generally a multimodal surface in the measurement points, is chosen as the sensitivity criterion. Actually, the random optimization technique is a trial and error procedure (random trials) in some sense. Therefore, what is lacking is a systematic way of finding the optimal measurement points in a distributed region. A method is proposed later in this chapter to fulfill this requirement. The optimal location of measurements for state estimation has been investigated by Thau [72], Cannon and Klein [25] and Yu and Seinfeld [77].

The following questions are studied in this chapter: 1) Do techniques exist for the estimation of parameters in partial differential equations from noisy data that are computationally efficient and involve no restrictions on the form of the differential equations or the data? 2) What is the effect of the level of measurement errors on the parameter estimates? 3) What is the effect of the number of spatial locations at which data are taken? 4) What is the effect of the number of times data is taken? 5) What is the effect of the initial parameter guesses on convergence of the algorithms? 6) How can one determine the best locations for a fixed number of measurements such that the resulting parameter confidence intervals are minimized?

To answer questions 1)- 5), parameter estimation schemes based on gradient optimization methods, quasilinearization, and a collocation method are tested extensively on three example systems: the estimation of the diffusivity in the heat equation, the estimation of the activation energy for a single reaction from steady state and transient plug flow reactor data, and the estimation of the permeabilities in a two-region reservoir model. To answer question 6) and to provide criteria for the earlier questions, a confidence interval analysis in conjunction with nonlinear programming to determine the optimal locations of measurements for constant parameter estimates in partial differential equations is presented.

2. Statement of the Problem

Let us consider the class of systems described by the partial differential equation

$$u_t(t,x) = f(t,x,u,u_x,u_{xx},k) \quad (1)$$

where $u(t,x)$ is the n -dimensional state vector, u_x and u_{xx} are partial derivatives with respect to x , and k is a p -dimensional vector of constant parameters. The initial state of the system is given by

$$u(0,x) = u_0(x) \quad x \in \Omega \quad (2)$$

where Ω denotes the fixed spatial domain of the system, and the boundary conditions are given by

$$g(t,u,u_x,k) = 0 \quad x \in \partial\Omega \quad (3)$$

In general the experimental data are related to the system state by a known functionality. Let the measurements on the system be represented by the m -dimensional ($m \leq n$) vector y and be made at R values of t, t_1, t_2, \dots, t_R and S spatial locations x_1, x_2, \dots, x_S . Then the measurements are related to the state by

$$\begin{aligned} y_{r,s} &= h(t_r, x_s, u(t_r, x_s)) + \eta_{r,s} \\ r &= 1, 2, \dots, R \\ s &= 1, 2, \dots, S \end{aligned} \quad (4)$$

where η is an m -dimensional vector of random error. Given the noisy observations $y_{r,s}$ we want to determine k such that the model matches the data in some optimal way. The least-square criterion has proven most useful in estimation applications, and thus we want to

determine k to minimize

$$J(k) = \sum_{r=1}^R \sum_{s=1}^S \|y_{r,s} - h(t_r, x_s, u(t_r, x_s, k))\|_{Q_{r,s}}^2 \quad (5)$$

where $u(t_r, x_s, k)$ is the solution of (1)-(3) for a given value of k and $Q_{r,s}$ in an $m \times m$ symmetric, positive semi-definite weighting matrix. Also, the norm $\|A\|_Q^2$ is defined by $A^T Q A$.

We should note that the problem formulated in (1)-(5) is by no means inclusive of all parameter estimation problems in partial differential equations, specifically because of the form of (1) and (4). Nevertheless, the formulation here is representative of the largest class of problems of chemical engineering interest (i.e., parabolic and hyperbolic systems). Moreover, the techniques used later on can be extended readily to elliptic systems and observations of forms other than (4).

3. Computational Methods

The basic problem is to locate the global minimum of $J(k)$ in the parameter space k . As such, the problem is analogous to that of the estimation of parameters in ordinary differential equations, a problem which has been more widely studied than that in distributed parameter systems. Wide experience in the estimation of parameters in ordinary differential equations indicates that gradient optimization and quasilinearization are two of the most efficient techniques and are thus candidates for the problem of parameter estimation in partial differential equations. In addition, methods which enable the solution

of nonlinear boundary value problems by trial function expansions are particularly attractive because of the explicit form of the solution. Furthermore, a close look at the formulation of the problem in the previous section shows that the parameter estimation problem is the same as the problem of optimal control. Therefore, the use of optimal control theory to determine the parameters would seem natural. Since optimal control will be explored in great detail in the estimation of spatially varying parameters later, the derivation and the application of this method will not be discussed here. We now outline these three methods.

3.1 Gradient Optimization Methods

Gradient optimization methods were developed to surmount the inherent difficulty associated with the nonlinear optimization problems. They are characterized by iterative algorithms for improving estimates of the parameters, or equivalently, the control variables, so as to come closer to satisfying the optimality conditions. An initial guess k^0 is improved iteratively by

$$k^{i+1} = k^i - \gamma [R]_{ki}^{-1} \left[\frac{\partial J}{\partial k} \right]_{ki}^T \quad (6)$$

where k^i is the value of k at the i th iteration, γ is a scalar step length, and R is a $p \times p$ matrix. The gradient of J is computed from

$$\left[\frac{\partial J}{\partial k} \right]^T = -2 \sum_{r=1}^R \sum_{s=1}^S \lambda^T(t_r, x_s) h_{u_{r,s}}^T [y_{r,s} - h(t_r, x_s, u(t_r, x_s, k))] \quad (7)$$

$$\lambda_t = f_u \lambda + f_{u_x} \lambda_x + f_{u_{xx}} \lambda_{xx} + f_k \quad (8)$$

$$\lambda(0,x) = 0 \quad x \in \Omega \quad (9)$$

$$g_u \lambda + g_{u_x} \lambda_x + g_k = 0 \quad x \in \partial\Omega \quad (10)$$

where $\lambda_{ij} = \partial u_i / \partial k_j$, the sensitivity coefficients of (1).

Various gradient methods differ from each other in the choice of γ and R . Here we do not intend to list exhaustively all gradient methods. Instead, four of the most common and efficient gradient techniques [5], namely, the method of steepest descent, the Newton-Raphson method, the Gauss-Newton method, and the Marquardt method will be presented.

The simplest gradient method is the method of steepest descent. In this method R is chosen as an identity matrix and γ is taken as an arbitrary step length. This method usually shows great improvements in the first few iterations but has poor convergence characteristics as the minimum of $J(k)$ is approached. To increase the rate of convergence, R is set equal to the Hessian matrix:

$$H = \frac{\partial^2 J}{\partial k^2} \quad (11)$$

and γ is chosen as one. This is the so-called Newton-Raphson method. Denoting the right-hand side of (8) by $F(u, u_x, u_{xx}, \lambda, \lambda_x, \lambda_{xx}, k)$ and the left-hand side of (10) by $G(u, u_x, \lambda, \lambda_x, k)$, the second-order gradient of J is computed from

$$\frac{\partial^2 J}{\partial k^2} = 2 \sum_{r=1}^R \sum_{s=1}^S \{ (h_u \lambda)^T Q_{r,s} (h_u x) - [y_{r,s} - h(t_r, x_s, u(t_r, x_s, k))]^T Q_{r,s} \frac{\partial^2 h}{\partial k^2} \} \quad (12)$$

$$\beta_t = F_u \lambda + F_{u_x} \lambda_x + F_{u_{xx}} \lambda_{xx} + F_\lambda \beta + F_{\lambda_x} \beta_x + F_{\lambda_{xx}} \beta_{xx} + F_k \quad (13)$$

$$\beta(0, x) = 0 \quad x \in \Omega \quad (14)$$

$$G_u \lambda + G_{u_x} \lambda_x + G_\lambda \beta + G_{\lambda_x} \beta_x + G_k = 0 \quad x \in \partial \Omega \quad (15)$$

where $\beta_{ij\ell} = \partial \lambda_{ij} / \partial k_\ell$.

The Newton-Ralphson method is the most efficient gradient method [33] because it possesses quadratic convergence properties as k gets closer to k^* , the true value of the parameter. Unfortunately, this great advantage is offset by the high cost of computing second order derivatives and it may have starting difficulties. This leads us to make use of simplification of the Newton-Ralphson method, such as the Gauss-Newton method. In the Gauss-Newton method R is set equal to the first term in the right-hand side of (12), in the hope that the difference between the observation and the solution of the model is small, then R is a good approximation to H . In this case the necessity to integrate (13)-(15) is avoided. Another modified Newton-Raphson method is the Marquardt method [57]. In this method we choose

$$R = (A + \beta C)^{-1} \quad (16)$$

where A is equal to the first term in the right-hand side of (12), β is a positive constant, and C is a diagonal matrix with $C_{ij} = |A_{ij}|$.

The choice of R in the form of (16) is to guarantee the positive definiteness of R provided that β is large enough.

Recently, a very attractive gradient method called the conjugate gradient method [17] which does not fit to the form of (6) has been used in optimization problems. This method has the advantages of the first-order and the second-order gradient methods without the requirement of calculating second order derivatives. However, in the use of the conjugate gradient method, it is required to find a scalar constant by a one-dimensional search. This means that we are required to solve (1)-(3) several times, and this is the most time consuming part of the parameter estimation, especially in the case of distributed parameter systems. Therefore, we will not discuss the conjugate gradient method further.

Equations (8)-(10) are called the sensitivity equations. We note that in the generating sensitivity coefficients the method of solving the sensitivity equations is superior to the conventional method by using a finite difference of the form

$$\lambda_{ij} = \frac{\partial u_i}{\partial k_j} = \frac{u_i(k_j + \Delta k_j) - u_i(k_j)}{\Delta k_j} \quad (17)$$

in terms of the computing effort and the accuracy where Δk_j is a small fraction of k_j . This is because the sensitivity equations generate the sensitivity coefficients exactly, instead of approximate ones, by means of the finite difference, and we can take the advantage of the similarity between the sensitivity equations and the state equations in the numerical calculations.

In this dissertation we will test only the steepest descent in the examples considered later. As pointed out before, γ is chosen as a scalar arbitrarily. However, it may sometimes be difficult to find a scalar γ for which the rate of convergence of the algorithm is reasonable, and thus it is advisable in those cases to compute γ as a $p \times p$ matrix by (11). In the two examples considered $p = 1$, so to obtain convergence, the choice of γ was a priori generally easy. Comparison of the two modes of determining γ yield approximately equal overall computing times.

3.2 Quasilinearization

By using finite difference approximations to the spatial derivatives in (1) and dividing the region Ω into N mesh points, (1) and (2) become

$$\frac{dU}{dt} = W(t, U, k) \quad (18)$$

$$u(0) = U_0 \quad (19)$$

where $U = (u_1^T, u_2^T, \dots, u_N^T)^T$, then nN -dimensional vector consists of the state vector at each of the N mesh points. In the case that (1) represents a hyperbolic system, the method of characteristics instead of finite difference approximations is used to transform the partial differential equation to a set of ordinary differential equations. This is due to the fact that the method of characteristics has at least two advantages when compared to the method of finite difference for reducing partial differential equations to ordinary differential

equations. First of all, a smaller number of ordinary differential equations must be solved, and secondly the characteristic differential equations constitute an exact representation of the partial differential equation.

In the form of (18) and (19), the quasilinearization, as initiated by Bellman and Kalaba [15] and used by Bellman et al. [13-14] and Lee [53], can be used to estimate the parameters. The quasilinearization approach for the parameter estimation can be formulated as follows:

(1) Adjoin to (18) and (19) the set of equations

$$\frac{dk}{dt} = 0 \quad (20)$$

with unknown initial conditions which are to be determined. The system we now deal with is the following

$$\frac{dz}{dt} = g(t, z) \quad (21)$$

$$z_i(0) = U_{i0} \quad i=1, \dots, nN \quad (22)$$

$$z_i(0) = ? \quad i=nN+1, \dots, nN+p \quad (23)$$

where $z^T = (U^T, k^T)$.

(2) Make an initial estimate of $k^{(0)}$ and solve (18) and (19). This first guessed solution is denoted by $z^{(0)}$.

(3) Linearize (21) to first order about $z^{(0)}$. The linearized version of (21) then becomes

$$\frac{dz^{(1)}}{dt} = g(z^{(0)}, t) + \left. \frac{\partial g}{\partial z} \right|_{z^{(0)}} [z^{(1)}(t) - z^{(0)}(t)] \quad (24)$$

(4) Apply the principle of superposition. The solution can be expressed in terms of the sum of a particular solution and p homogeneous solutions

$$z^{(1)}(t) = z_p^{(1)}(t) + \sum_{i=1}^p k_i^{(1)} \phi_{i+nN} \quad (25)$$

where ϕ is the fundamental matrix, ϕ_i is the i th column of ϕ , $z_p^{(1)}(t)$ is the particular solution, and $k_i^{(1)}$ represent the new estimates of k_i , $i=1, \dots, p$. Notice that we assume the initial conditions U_0 are known exactly.

(5) Determine $k^{(1)}$ by minimizing the performance index J , i.e., solve the following equations

$$\frac{\partial J}{\partial k_i} = 0 \quad i=1, \dots, p \quad (26)$$

to determine $k^{(1)}$.

(6) Return to step (2) with $z^{(1)}(t)$ in place of $z^{(0)}(t)$ if the specified convergence criteria is not satisfied. The convergence criterion for both steepest descent and quasilinearization is

$$|(k_\lambda^{j+1} - k_\lambda^j)/k_\lambda^j| \leq \epsilon, \quad \lambda=1, \dots, p.$$

3.3 Parameter Estimation Using Collocation

It is well known that the most time consuming part of parameter estimation for distributed systems is the solution of the state and sensitivity equations. In order that a method is to be effective, the computational time should be short. Several methods have been proposed as cited above to reduce the partial differential equation to a set of

ordinary differential equations or a set of algebraic equations so that the computing time can be shortened. However, these methods are not promising for the wide class of distributed parameter systems. In this section trial-function expansions, or more specifically, the collocation methods, are used to transform the partial differential equations into a set of ordinary differential equations or a set of algebraic equations.

In these methods the unknown solution is expanded in a series of known functions of position with undetermined, arbitrary functions of time. The expansion coefficients are normally determined by variational principles [39] or by weighted-residual methods [37,38]. Since the latter are more widely applicable, the weighted-residual methods are discussed here. In the method of weighted residuals the unknown functions of time are determined by satisfying the partial differential equations in some average sense, such as Galerkin's method, the least squares method, or the method of moments or pointwise sense, such as the collocation methods. In determining the unknown functions, the collocation methods are most direct, requiring only evaluations of the residual, whereas the other methods require integrations. Furthermore, for problems involving chemical reactions with a nonlinear rate expression, only the collocation methods are feasible, since the other methods require evaluation of complicated integrals involving exponential functions [36]. Therefore, the collocation methods will be used in this study.

If the differential equation and boundary conditions are written

$$L^{\Omega}(u(x,t)) = 0 \quad \text{in } \Omega \quad (27)$$

$$L^{\partial\Omega}(u(x,t)) = 0 \quad \text{on } \partial\Omega \quad (28)$$

then $u(x,t)$ is approximated by a series expansion

$$u^{\ell}(x,t) = \sum_{i=1}^{\ell} a_i(t) f_i(x) \quad (29)$$

containing ℓ known functions $f_i(x)$ and ℓ unknown functions $a_i(t)$. The unknown functions are then determined by applying (1) and (2) or (3) at each of the ℓ selected points in Ω . There are three classes of collocation methods, namely, interior, boundary and mixed [75]. Interior collocation requires a $u^{(\ell)}$ which satisfies the boundary conditions identically, and the function is adjusted to satisfy (1) and (2) at ℓ points in Ω . Boundary collocation requires a $u^{(\ell)}$ which satisfies (1) and (2) identically and is adjusted to satisfy (3) at ℓ points on $\partial\Omega$. Mixed collocation requires a $u^{(\ell)}$ which does not satisfy (1), (2) or (3) and is adjusted to satisfy (1), (2) and (3) at ℓ points.

The choice of approximating functions can be crucial in applying the collocation method. At present there is no way generally available to choose the best approximating functions for a given problem systematically and uniquely. The choice of a trial solution is up to the ingenuity and experience of the investigator. The more that is known about the expected behavior of a solution, such as symmetry properties, the more intelligently can the trial solution be set up. However, two guidelines which may be used to help in the choice of

trial functions are: to choose the trial functions to be members of a complete set of functions which satisfy the boundary conditions and to choose the trial functions to be orthogonal in Ω [63].

Once the partial differential equation has been transformed into a set of ordinary differential equations or algebraic equations by the collocation method, the method of steepest descent or the other methods can be used to estimate the parameters in the resulting equations. Since the collocation method will yield an approximate solution which is an explicit function of spatial variables, this makes it easier to determine the optimal measurement locations for the parameter estimation in distributed processes. This may be considered as a very desirable feature of this method. This will be seen in the next section.

4. Accuracy of Constant Parameters Estimated in Partial Differential Equations

In this section the technique developed by Rosenbrock and Storey for analyzing the accuracy of constant parameters estimated in ordinary differential equations is extended to parameter estimates in partial differential equations. The question is: given several estimated values of a certain parameter, for example, as the result of different methods or different sets of data from various experiments, which estimate is most reliable? The question is then reduced to a comparison of confidence intervals for each parameter estimate, or, equivalently, variances of the error in the parameter estimates. The application of this analysis in the optimal location of measurements is also discussed here.

4.1 Theory

The true value k^* and the estimated value \hat{k} are related by

$$\hat{k} = k^* + \kappa \quad (30)$$

where κ is the error in the estimate \hat{k} . In order to carry out the analysis it is necessary to assume certain statistical properties of the measurement errors. For simplicity we assume the errors of the individual data points are independent and normally distributed with mean zero and covariance matrix $M_{r,s}$. Confidence intervals on \hat{k} can be obtained from $P = E[\kappa \kappa^T]$, the covariance of the estimate errors. The determination of P proceeds as follows when the value k^* of \hat{k} that minimizes J has been found and the initial conditions are known exactly. Consider the function $J(k^* + \kappa)$ defined by (5). Expanding $J(k^* + \kappa)$ in a Taylor series, and keeping only terms of first order in κ , we obtain

$$\begin{aligned} J(k^* + \kappa) &= \sum_{r=1}^R \sum_{s=1}^S \{y_{r,s} - h(t_r, x_s, u(t_r, x_s, k^*)) \\ &\quad - G_{r,s} \lambda_{r,s} \kappa\}^T Q_{r,s} \{y_{r,s} - h(t_r, x_s, u(t_r, x_s, k^*)) - G_{r,s} \lambda_{r,s} \kappa\} \\ &= \sum_{r=1}^R \sum_{s=1}^S \{\eta_{r,s} - G_{r,s} \lambda_{r,s} \kappa\}^T Q_{r,s} \{\eta_{r,s} - G_{r,s} \lambda_{r,s} \kappa\} \quad (31) \end{aligned}$$

where

$$\begin{aligned} G_{r,s} &= (G_{ij})_{r,s} = \left(\frac{\partial}{\partial u_j} h_i(t_r, x_s, u(t_r, x_s, k^*)) \right), \\ &\quad i=1, \dots, m \\ &\quad j=1, \dots, n \quad (32) \end{aligned}$$

$$\lambda_{r,s} = (\lambda_{ij})_{r,s} = \left(\frac{\partial}{\partial k_j} u_i(t_r, x_s, k^*) \right), \quad \begin{matrix} i=1, \dots, n \\ j=1, \dots, p \end{matrix} \quad (33)$$

Notice that $\lambda_{r,s}$ are the solutions of (8)-(10). Let κ be chosen to make $J(k^* + \kappa)$ a minimum and perform the minimization, obtaining

$$\sum_{r=1}^R \sum_{s=1}^S \lambda_{r,s}^T G_{r,s}^T Q_{r,s} \{ \eta_{r,s} - G_{r,s} \lambda_{r,s} \kappa \} = 0 \quad (34)$$

or

$$H \kappa = \sum_{r=1}^R \sum_{s=1}^S \lambda_{r,s}^T G_{r,s}^T Q_{r,s} \eta_{r,s} \quad (35)$$

where H is a symmetric matrix and defined by

$$H = \sum_{r=1}^R \sum_{s=1}^S \lambda_{r,s}^T G_{r,s}^T Q_{r,s} G_{r,s} \lambda_{r,s} \quad (36)$$

Now we are in a position to calculate the expected value P of $\kappa \kappa^T$. By (35)

$$E[H \kappa \kappa^T H] = E \left[\sum_{r=1}^R \sum_{r'=1}^R \sum_{s=1}^S \sum_{s'=1}^S \lambda_{r,s}^T G_{r,s}^T Q_{r,s} \eta_{r,s} \eta_{r',s'}^T Q_{r',s'} G_{r',s'} \lambda_{r',s'} \right] \quad (37)$$

where $E[\]$ denotes the expectation operator. Since the errors of the individual data points are independent and normally distributed with mean zero and covariance matrix $M_{r,s}$, (37) becomes

$$HPH = \sum_{r=1}^R \sum_{s=1}^S \lambda_{r,s}^T G_{r,s}^T Q_{r,s} M_{r,s} Q_{r,s} G_{r,s} \lambda_{r,s} \quad (38)$$

This equation determines P if H is nonsingular.

In the preceding analysis the weighting matrix $Q_{r,s}$ was chosen arbitrarily. A natural conjecture at this point is whether or not one can find a weighting matrix which is the best in some sense. It is well known that the choice $M_{r,s}^{-1}$, the inverse of the covariance matrix of the errors of data, for the weighting matrix yields a minimum error covariance matrix [34,66]. Due to this property, we shall henceforth take $M_{r,s}^{-1}$ as a weighting matrix for the analysis of the accuracy. Using $M_{r,s}^{-1}$ in the place of $Q_{r,s}$, we have

$$P = H^{-1} = \left[\sum_{r=1}^R \sum_{s=1}^S \lambda_{r,s}^T G_{r,s}^T M_{r,s}^{-1} G_{r,s} \lambda_{r,s} \right]^{-1} \quad (39)$$

By (35) the error in the estimated errors of the parameters is normally distributed with zero mean and covariance matrix P . Thus the variance of the linear combination $b^T \kappa$ of κ is

$$\sigma_b^2 = b^T P b \quad (40)$$

where b is a unit p -dimensional vector. Then the confidence interval associated with $b^T \hat{\kappa}$ will be the interval $b^T \hat{\kappa} - \alpha \sigma_b$ to $b^T \hat{\kappa} + \alpha \sigma_b$ [51]. The value of α depends on the choice of confidence level. For example, if we assert that $b^T \kappa^*$ lies in the range $b^T \hat{\kappa} + 2\sigma_b$, we shall be right in about 95.45% of cases in a large number of similar estimations. The confidence interval for the individual elements of $\hat{\kappa}$ is determined by setting $b_i = 1$; $b_j = 0$, $j \neq i$. This gives

$$\sigma_{k_i}^2 = P_{ii} \quad (41)$$

It must be noted that the confidence interval corresponding to a given confidence level is not unique and the upper and lower confidence limits are not necessary to be equidistant from $b^T \hat{k}$. For instance, with the same confidence level, 95.45%, we can assert that $b^T k^*$ lies in the interval $b^T \hat{k} + 1.806\sigma_b$ to $b^T \hat{k} - 2.326\sigma_b$. We observed that in the first case the interval length is $4\sigma_b$, while in the second case the interval length is $4.132\sigma_b$. Thus, in general, we choose the first case in which the upper and lower confidence limits are equidistant from $b^T \hat{k}$.

It should be pointed out that in the calculations of $\lambda_{r,s}$ and $G_{r,s}$, \hat{k} is used in place of k^* . This is necessary because k^* is unknown, and \hat{k} is the best estimate which we have of k^* . However, this approximation does not affect the accuracy of the analysis because the errors caused by this substitution are second order in κ . This is the same order as errors already ignored in the linearization of $J(k^* + \kappa)$.

It is interesting to note that the nonsingularity of H is a necessary condition for the local observability of parameters or local identifiability of parameters. This condition is equivalent to the condition given by Hwang and Seinfeld [45], Haddad and Cruz [43], and Tse [73]. If H^{-1} does not exist, one or more elements of P are infinite, indicating one or more parameters cannot be estimated from the given data. Thus, the local observability depends on n, m, R, S and the location of the measurements x_1, x_2, \dots, x_S . The concept of local observability or identifiability of parameters is very important because most of the nonlinear parameter estimation algorithms are of the type of local variation.

4.2 Applications

There are at least two different ways the foregoing analysis can be employed. The first way is simply the determination of the reliability of parameters estimated from noisy data. Another use for this analysis, however, is in the planning of experiments or, more specifically, the determination of the optimal location of measurements in a distributed region. In the former case, this analysis is used to determine the accuracy of kinetic parameters estimated from batch and integral reactor data for four fundamental reactions, and the reliability of reservoir parameters from history matched drill stem tests. The results are presented in Appendices II-B and II-C. For the latter case a method of determining the optimal location of measurement points is proposed in this section.

The problem which we are faced with in the planning of experiments, the objective of which is the estimation of unknown parameters appearing in the system (1)-(3) based on the observations (4), is at what locations, i.e., x_1, \dots, x_s , should the measurements be taken such that the highest accuracy of the estimated parameters is achieved. Since $P = H^{-1}$ represents the covariance of estimated errors, the matrix P will provide useful information on the choice of the optimal measurement points. Several criteria which are some function of the error covariance matrix P have been proposed in the case in which the model consists of a set of algebraic rather than differential equations. Among these are the following:

(a) Maximization of the minimum eigenvalue of H with respect to measurement points [4]. Note that the measurement "points" can be referred to as the locations in spatial domain, some particular times in time domain or some independent variables such as temperature, etc.

(b) Minimization of the determinant of the matrix P or the product of its eigenvalues, or maximization of the determinant of the matrix H or the product of its eigenvalues with respect to the measurement points [16].

(c) Minimization of the trace of the matrix P or $1/\text{trace } H$ with respect to the measurement points [27]. We note that the trace of P is the sum of the variances of the components of k . Aoki and Staley [3] show that in the multi-parameter case the maximization of $\text{tr } H$ is asymptotically equivalent to the minimization of $\text{tr } P$.

Before proceeding to choose the criterion, we assume that we are interested in all P parameters. For the single parameter case x_1, \dots, x_s are chosen to minimize P or maximize H directly, since P or H is a scalar. It is clear that the best choice for a criterion of optimality is not obvious for the multi-parameter problem and we are not to expect that these three criteria will lead to the same optimal measurement locations. Since it is assumed that the values of all the parameters are of equal interest to the experimenters, a reasonable criterion is that it should minimize the volume of the joint confidence region of the parameters. This leads us to choose the criterion (b) as a criterion of optimality because the square root of the determinant of H is inversely proportional to the volume of the

joint confidence region and note that $\det H = 1/\det P$. This criterion may possess the undesirable characteristic that the resulting shape of the joint confidence region may be a highly elongated hyper-ellipsoid in spite of the fact that the minimum volume has been achieved. In this situation some of the P parameters may be ill-determined. We note that the criterion (c) also possesses this characteristic. However, the ability of the criterion (b) to lead to precise parameter estimates in a small number of data has been demonstrated by Kittrell et al. [52], Graham and Stevenson [42], Sater and Stevenson [67], and Juusola et al. [49]. In addition, the criterion (b) is more tractable analytically or numerically than the criteria (a) and (c). Thus, the criterion (b) will be used in this study.

In order to make the problem more manageable, the following assumptions are made:

- (a) The errors in measurement are random. On the other hand, we do not know in advance where we can get the most accurate observations.
- (b) The number of times at which data are taken is fixed. If the observations are taken at some particular spatial locations continuously, the period over which the observations are made is fixed.
- (c) The number of measurement locations is fixed.
- (d) A method exists to estimate the parameters.

The criterion will be independent of the values of parameters if the solution of (1)-(3) is a linear function of parameters. In general, the solution of (1)-(3) is nonlinear in parameter k , therefore the criterion is a function of parameters. This means that the choice of

the optimal locations depends on the actual values of the P parameters. This is the reason we make the assumption that there exists a method to estimate the parameters. In fact if we know nothing about the parameters, we cannot design the experiments for the estimation of parameters. Due to the dependence of the criterion on the values of parameters, an iterative method seems to be the most plausible one to solve this problem. We use the preliminary estimate values of parameters \hat{k} instead of the true values of parameters k^* in the criterion to determine the optimal locations, the results of which are used to design the experiments and obtain the new estimates of parameters, and so on.

In summary, the problem of optimal locations of measurements can be stated as follows: Determine the S locations (x_s) , $s=1, \dots, S$ to maximize $|H|$ subject to the constraints

$$x_s \in \Omega + \partial\Omega \quad s=1, \dots, S \quad (42)$$

$$|x_i - x_j| \geq \epsilon \quad i \neq j \quad (43)$$

where ϵ is some prescribed constant. The first constraint states that the locations be placed on the boundary or within the boundary. The second constraint is attributed to physical limitations. This means that we cannot place two sensors too close. As posed above, this is a nonlinear programming problem. The gradient projection method developed by Rosen [65] can be applied to solve this problem.

We can now formulate the following algorithm for solving this problem:

(a) Make an initial estimate of k^0 and solve (1)-(3) and (8)-(10).

(b) Assume values for the S observation points (x_s) , $s=1, \dots, S$. Denote these initial guesses by (x_s^0) , $s=1, 2, \dots, S$.

(c) Compute $|H|$ by (39). In the calculation of $|H|$, it is assumed that $M = I\sigma^2$ where σ^2 denotes the common variance of each observation. Denote this value of $|H|$ by $|H^0|$.

(d) Use a gradient projection method to determine the optimal locations x_s , $s=1, \dots, S$. Note that this is the optimal solution for $k = k^0$. Denote these new points by (x_s') , $s=1, \dots, S$. In the process of using the gradient projection method we are required to calculate the gradient $\partial|H|/\partial x_s$ several times. There is not any difficulty in calculating this gradient because $|H|$ is a function of λ at the observation points and we have already calculated the value of λ over all the whole domain in (a). The gradient is calculated by the finite difference of the form

$$\frac{\partial|H|}{\partial x_i} \equiv \frac{|H|(x_1^0, \dots, x_i^0 + \Delta x_i, \dots, x_S^0) - |H|(x_1^0, \dots, x_i^0)}{\Delta x_i} \quad (44)$$

where Δx_i is a small fraction of x_i .

(e) Take measurements at (x_s') , $s=1, \dots, S$ and estimate the parameters based on these new observations. Denote the new estimates by k' .

(f) Return to step (a) and replace k^0 by k' and (x_s^0) by (x_s') , $s=1, \dots, S$.

(g) Continue iterating until subsequent changes in (x_s) , $s=1, \dots, S$ are less than a certain level,

$$\frac{|x_s^{i+1} - x_s^i|}{x_s^i} \leq \xi \quad s=1, \dots, S \quad (45)$$

where ξ is a preset convergence criterion.

A simple sub-optimal way called "imbedding" technique proposed by Jamshidi [47] and employed by Yu and Seinfeld [77] to determine the optimal measurement points for the state estimation can be applied to solve this problem.

The method proposed in this section can be applied to determine the optimal input (assumed the measurement locations are fixed), for instance the heat flux, for constant parameter estimation as well. This problem has been treated for estimating constant parameters in ordinary differential equations or difference equations by Kalaba and Spingarn [50], Mehra [60], Aoki and Staley [3], and Nahi and Wallis [62].

5. Examples

In this section a few computational examples are presented to supplement the theoretical discussions given above.

5.1 Example 1: Estimation of the Diffusivity in the Heat Equation

We consider a system governed by the heat equation

$$u_t(t,x) = ku_{xx}(t,x) \quad (46)$$

$$u(0,x) = \sin \pi x \quad 0 \leq x \leq 1 \quad (47)$$

$$u(t,0) = u(t,1) = 0 \quad 0 \leq t \leq T \quad (48)$$

in which observations of the state are made at R times and S spatial

Locations,

$$y_{r,s} = u(t_r, x_s) + (\text{errors}) \quad (49)$$

$$r = 1, 2, \dots, R$$

$$s = 1, 2, \dots, S$$

The noisy measurements are generated artificially by

$$y_{r,s} = u^*(t_r, x_s) (1 + \sigma \text{ Gauss}(a, b)) \quad (50)$$

where $u^*(t_r, x_s)$ is the exact solution of (46)-(48) with k equal to the assumed true value of one, and $\text{Gauss}(a, b)$ is a normally distributed random variable with mean a and standard deviation b . The problem is to determine k to minimize

$$J(k) = \sum_{r=1}^R \sum_{s=1}^S (y_{r,s} - u(t_r, x_s, k))^2 \quad (51)$$

where $Q_{r,s}$ has been taken as 1. Each of the six questions in the beginning of this chapter is studied in this example.

5.1.1. Steepest Descent and Quasilinearization

The effect of the level of measurement error was studied with $R = 200$, $S = 9$, $N = 9$, $k^0 = 0.5$, $T = 0.2$, $a = 0$ and $b = 0.3$. The convergence criterion used was $\epsilon = 0.005$ and in steepest descent $\gamma = 0.5$. The results for $\sigma = 0.9$, 0.3 and 0.5 are shown in Table II-1. Neither method is overly sensitive to the level of measurement error, with approximately two percent maximum error in k . This result is encouraging, although necessary, for the general use of both methods. Steepest descent is slightly more accurate and somewhat faster

Table II-1. Effect of Level of Measurement Error on \hat{k}

σ		Steepest Descent	Quasilinearization
0.1	\hat{k}	1.01558	0.97934
	iterations	14	4
	% error	1.56	2.07
	comp. time, sec.	16.40	15.24
0.3	\hat{k}	1.01733	0.97894
	iterations	14	6
	% error	1.73	2.11
	comp. time, sec.	16.01	18.67
0.5	\hat{k}	1.01902	0.97050
	iterations	14	8
	% error	1.90	2.95
	comp. time, sec.	16.31	23.03

computationally, although the differences are not significant. Computing times reported are for an IBM 360-75.

The effect of the number of times R at which data is taken was studied next with $S=9$, $N=9$, $T=0.2$, $k^0=0.5$, $a=0$, $b=0.3$, $\sigma=0.3$, $\gamma=0.5$, and $\epsilon=0.005$. The results for $R=200$, 100, 20 and 10 are shown in Table II-2. For small values of R it appears that the accuracy of steepest descent deteriorates faster than that of quasilinearization. At large values of R computing times are roughly comparable for the two methods, although as R decreases, steepest descent becomes more than twice as fast. A constant value of γ was used for the results in Tables II-1 and II-2. As we outlined, γ can also be computed from

Table II-2. Effect of Number of Measurement Times R on \hat{k}

R		Steepest Descent	Quasilinearization
200	\hat{k}	1.01733	0.97894
	iterations	14	6
	% error	1.73	2.11
	comp. time, sec.	16.01	18.67
100	\hat{k}	1.02600	0.98176
	iterations	14	5
	% error	2.60	1.82
	comp. time, sec.	10.61	14.56
20	\hat{k}	1.02058	0.98314
	iterations	10	6
	% error	2.06	1.69
	comp. time, sec.	6.57	15.44
10	\hat{k}	1.07617	0.97324
	iterations	11	13
	% error	7.62	2.68
	comp. time, sec.	6.64	18.33

(11). The $R = 20$ case in Table II-2 was repeated using the second variation (11), with $k = 0.99875$ in four iterations and 6.39 seconds. It thus appears that γ can be chosen arbitrarily or computed from (11) with roughly similar results. Use of (11) requires the extra computations of (13)-(15) and thus will not save computing time substantially over a guess of γ based on the relative magnitudes of k and J .

The effect of the number of spatial locations S at which data is taken and the location of these measurements was studied with $R=20$, $k^0=0.5$, $T=0.2$, $N=9$, $\gamma=0.5$, $\sigma=0.3$, $a=0$, and $b=0.3$. The results for $S=9$, 2 and 1 are shown in Table II-3; for $S=2$, $x_1=0.1$ and $x=0.4$, and for $S=1$, $x=0.1$, 0.3 and 0.5. The last three cases were included to study the effect of the location of the single measurement if only one can be used. We see that there is essentially no difference between \hat{k} for $S=9$ and $S=2$, and, in fact, \hat{k} for $S=2$ are slightly better, a fact which can only be attributed to the different shape of the $J(k)$ surface and the particular iterations. Thus, in this system $S=2$ is sufficient for highly accurate \hat{k} . Also we note that locating the measurement at 0.5 appears to yield the best estimates. We will consider this point shortly.

Finally, the effect of the initial guess k^0 was examined. In the steepest descent it is necessary to adjust γ , or use (11), when initial guesses are poor. Although we will not present the results, convergence was obtained for k^0 as small as 0.0001 and as large as 2.5 in both methods. As k^0 is poorer, the final estimates are not as accurate.

5.1.2 Interior Collocation

Of the three collocation methods, the interior collocation is more versatile, since it can be used for nonlinear differential equations. Thus, the interior collocation will be used in this study. The

Table II-3. Effect of Number and Location of Measurements on \hat{k}

S		Steepest Descent	Quasilinearization
9	\hat{k}	1.02058	0.98314
	iterations	10	6
	% error	2.06	1.69
	comp. time, sec.	6.57	15.44
2	\hat{k}	1.01928	0.99198
	iterations	7	5
	% error	1.93	0.80
	comp. time, sec.	5.26	12.71
1 ($x_1=0.1$)	\hat{k}	0.86169	0.93997
	iterations	7	5
	% error	13.83	6.00
	comp. time, sec.	4.80	12.22
1 ($x_1=0.3$)	\hat{k}	1.06112	0.93712
	iterations	7	5
	% error	6.11	6.29
	comp. time, sec.	4.51	12.13
1 ($x_1=0.5$)	\hat{k}	1.03217	0.92916
	iterations	6	5
	% error	3.22	7.08
	comp. time, sec.	4.53	12.43

interior collocation requires that the approximate function satisfy the boundary conditions identically and be adjusted to satisfy the partial differential equations and initial condition at a number of points. We assume the approximation function

$$u(t,x) = A(t) + B(t)\left(\frac{1}{2} - x\right)^2 + C(t)\left(\frac{1}{2} - x\right)^4 \quad (52)$$

In order to satisfy (48) we choose

$$A(t) = -\frac{1}{4} B(t) - \frac{1}{16} C(t) \quad (53)$$

and (52) becomes

$$u(t,x) = -\frac{1}{4} B(t) - \frac{1}{16} C(t) + B(t)\left(\frac{1}{2} - x\right)^2 + C(t)\left(\frac{1}{2} - x\right)^4 \quad (54)$$

Let us use $x = \frac{1}{5}$ and $x = \frac{1}{2}$ as collocation points. Evaluating (54) at $t = 0$ and using (47) we find $B(0) = -4.90625$ and $C(0) = 3.625$. Evaluating (54) for $t > 0$ we obtain

$$\frac{dB(t)}{dt} = 4.5k B(t) + 18.75k C(t) \quad (55)$$

$$\frac{dC(t)}{dt} = 50k B(t) - 75k C(t) \quad (56)$$

the solutions of which are

$$B(t) = 0.053e^{-60.6kt} - 4.969e^{-9.9kt} \quad (57)$$

$$C(t) = 0.184e^{-60.6kt} + 3.809e^{-9.9kt} \quad (58)$$

Comparison of (54) with (57) and (58) to the previously used finite difference solution revealed that the collocation solution is slightly more

accurate.

The value of k that minimizes (51) can be readily determined using (54), (57) and (58). We obtain $\hat{k} = 0.99120$, as compared to 1.03217 and 0.92916 for the conditions of the last entry in Table II-3. It thus appears that partial differential equation solution methods based on trial-function expansions may be not only a desirable alternative to finite differences but also a powerful tool for parameter estimation.

5.1.3 Confidence Interval Analysis and Optimal Measurement Location

A confidence interval analysis for the estimation of k in (46)-(48) was carried out. If it is assumed that $M_{r,s} = \sigma^2 I$, then the variance of the error in estimates of k is given by

$$P = \sigma_k^2 = \sigma^2 \left[\sum_{r=1}^R \sum_{s=1}^S (-\pi^2 t_r e^{-k\pi^2 t_r} \sin \pi x_s)^2 \right]^{-1} \quad (59)$$

It can be seen that P does not become infinite on $0 < x < 1$ and that the system is observable. If, however, the initial condition (47) were $u_0(x) = \sin 4\pi x$, the variance of the error in k is

$$\sigma_k^2 = \sigma^2 \left[\sum_{r=1}^R \sum_{s=1}^S (-16\pi^2 t_r e^{-16k\pi^2 t_r} \sin 4\pi x_s)^2 \right]^{-1} \quad (60)$$

Now, if the measurements are only at the nodes 0.25, 0.50, 0.75, $\sigma_k^2 \rightarrow \infty$ and the system is unobservable. One measurement at a point other than a node will make the system observable.

Figure II.1 shows the dimensionless variance $\sigma_k^2/k^2\sigma^2$ vs. kT for various values of R and $S = 9$. A minimum value of the dimensionless variance exists for every R at $kT = 0.156$. Given several values of k from different estimation schemes (and not knowing the true value), one can determine the most accurate value from Figure II.1. Figure II.2 shows the relationship between $\sigma_k^2/k^2\sigma^2$ and R as a function of kT . The dimensionless variance is a strong function of R for $R < 20$ and a weak function of R for larger values of R . This is consistent with the results in Table II-2.

Confidence intervals for the estimates of k can also be determined by performing a large number of computer experiments which differ only by the set of experimental errors generated. Such an analysis appears in Appendix II.A.

Since the parameter is a scalar, the problem of selecting an optimal measurement location reduces to the minimization of P or σ_k^2 by choice of x_1, \dots, x_S . For this particular example, the choice of optional measurement location is independent of the value of k . Thus, sequential experimental design is not necessary. To illustrate, first let us consider one measurement case, i.e., $S = 1$. For this case, the variance of the error in estimate k is given by

$$P = \sigma_k^2 = \sigma^2 \left[\left\{ \sum_{r=1}^R (-\pi^2 t_r e^{-k\pi^2 t_r})^2 \right\} \sin^2 \pi x_1 \right]^{-1} \quad (61)$$

Clearly, the minimum value of σ_k^2 is achieved at $x_1 = 0.5$. However, for the case of two measurements the optimal location is not so obvious. Let us consider the optimal location of two observations in

two cases: (i) $u(0,x) = \sin \pi x$, and (ii) $u(0,x) = \sin 2\pi x$.

In case (i) it is required to determine x_1 and x_2 to minimize

$$P = \sigma_k^2 = \sigma^2 \left[\left\{ \sum_{r=1}^R (-\pi^2 t_r e^{-k\pi^2 t_r})^2 \right\} (\sin^2 \pi x_1 + \sin^2 \pi x_2) \right]^{-1} \quad (62)$$

subject to the constraints

$$1 - x_1 > 0 \quad (63)$$

$$x_2 > 0 \quad (64)$$

$$x_1 - x_2 - 0.1 \geq 0 \quad (65)$$

Now apply the gradient projection method and start from $x_1 = 0.85$ and $x_2 = 0.75$. The optimal measurement points are found at $x_1 = 0.55$ and $x_2 = 0.45$. This is a constrained minimum, i.e., optimal points lie on the boundary. The optimal locations of measurements are found at $x_1 = 0.50$ and $x_2 = 0.40$ or $x_2 = 0.60$ if the "imbedding" technique is employed. Obviously, this solution is not the optimum.

In case (ii), it is required to choose x_1 and x_2 to minimize

$$P = \sigma_k^2 = \sigma^2 \left[\left\{ \sum_{r=1}^R (-4\pi^2 t_r e^{-4\pi^2 k t_r})^2 \right\} (\sin^2 2\pi x_1 + \sin^2 2\pi x_2) \right]^{-1} \quad (66)$$

subject to (63)-(65). Apply the gradient projection method again and start from $x_1 = 0.55$ and $x_2 = 0.45$. The optimal locations are $x_1 = 0.75$ and $x_2 = 0.25$. This is an interior minimum, i.e., optimal locations are in the interior.

From column 3 of Table II-3 we can see that the percent error in the estimate of k is 13.83% for one observation at $x_1 = 0.1$ and 3.22% for one measurement at $x_1 = 0.5$ which is the optimal location. The results clearly show the advantage of taking the measurements at the optimal location.

5.2 Example 2: Estimation of the Activation Energy for a Single Reaction

Let us consider the problem of estimating the activation energy for a single reaction from steady state and transient data in an adiabatic plug flow reactor. If the reaction is irreversible and first order, physical properties are constant, and the effect of radial gradients and turbulent axial diffusion are negligible, the transient behavior of the reactor is described in dimensionless terms by

$$u_{1t} + u_{1x} = -\exp(ku_2/(\phi + u_2))u_1 \quad (67)$$

$$u_{2t} + u_{2x} = \exp(ku_2/(\phi + u_2))u_1 \quad (68)$$

$$u_1(0,x) = u_{1_0}(x) \quad (69)$$

$$u_2(0,x) = u_{2_0}(x) \quad (70)$$

$$u_1(t,0) = \bar{u}_1(t) \quad (71)$$

$$u_2(t,0) = \bar{u}_2(t) \quad (72)$$

$u_{1_0}(x)$ and $u_{2_0}(x)$ are the steady state solutions to (67) and (68)

with $\bar{u}_1 = 1$ and $\bar{u}_2 = 0$. We assume measurements of both concentrations u_1 , and temperature u_2 , may be made at R times and S locations,

$$y_{1,r,s} = u_1(t_r, x_s) + (\text{errors}) \quad (73)$$

$$y_{2,r,s} = u_2(t_r, x_s) + (\text{errors}) \quad (74)$$

We desire to estimate the dimensionless activation energy k from both steady state and transient experimental data. Artificial measurements are generated by

$$y_{i,r,s} = u_i^*(t_r, x_s) [1 + \sigma \text{Gauss}(a,b)], \quad i=1,2 \quad (75)$$

where $u^*(t,x)$ is the solution of (67)-(72) with $\phi = 7.1203$ and the assumed true value of $k = 30.1588$, values taken from Crider and Foss [32]. In the transient case $\bar{u}_1(t) = 1 + 0.005t$ and $\bar{u}_2(t) = 0$. In practice it is easier to measure temperature than concentration, so in addition to the questions raised in the beginning of the paper we want to study the effect of the number of state variables measured. For all cases $a = 0$ and $b = 0.3$ in (75).

Let us first consider the estimation of k from steady state temperature measurements only. Since the system is now governed by one ordinary differential equation, the steepest descent and quasilinearization methods need not be detailed. First, we examine the effect of the level of measurement error. The results for $S = 20$ ($x_1 = 0.025, \dots, x_{20} = 0.50$) and $k^0 = 15$ are shown in Table II-4 for $\sigma = 0.1, 0.3$ and

0.5. Again the results are relatively unaffected by the level of error. Computing times for all the steady state examples were two to three seconds. The effect of the number of locations S was studied next for $\sigma = 0.3$, $k^0 = 15$, the results of which are shown in Table II-5. For $S = 5$, $x_1 = 0.1, \dots, x_5 = 0.5$, and for $S = 3$, $x_1 = 0.2$, $x_2 = 0.35$ and $x_3 = 0.50$. As S decreases the estimate errors increase, as expected.

Table II-4. Effect of Level of Measurement Error on \hat{k} (Steady State, Temperature Measurements Only)

σ		Steepest Descent	Quasilinearization
0.1	\hat{k}	30.33215	29.96521
	iterations	5	5
	% error	0.58	0.64
0.3	\hat{k}	30.10222	30.11076
	iterations	4	4
	% error	0.19	0.16
0.5	\hat{k}	29.46460	30.07391
	iterations	8	4
	% error	2.30	0.28

It is interesting to explore the advantage of measuring the concentration in addition to the temperature when the number of measurement locations is small[†]. If the concentration is also measured in the $S = 5$

[†]Since concentration and temperature are not independent in the adiabatic steady state case, this results in $m > n$.

case in Table II-5, we obtain $k = 30.07054$, an error of 0.29%, by steepest descent. If concentration is measured in the $S = 3$ case in Table II-5, $k = 30.51721$, an error of 1.19% by quasilinearization. Thus, highly accurate estimates can be obtained by measuring both temperature and concentration at a few points as well as by measuring only temperature at many points.

Table II-5. Effect of the Number of Measurements on \hat{k} (Steady State Temperature Measurements Only)

S		Steepest Descent	Quasilinearization
20	\hat{k}	30.10222	30.11076
	iterations	4	4
	% error	0.19	0.16
5	\hat{k}	28.92407	29.92207
	iterations	18	8
	% error	4.10	0.78
3	\hat{k}	28.57324	28.91307
	iterations	20	4
	% error	5.03	4.15

Now let us consider the estimation of k from transient experimental data. Of interest will be comparisons of the accuracy of \hat{k} and computing times for transient vs. steady state experimental data. As before, we first consider the effect of the level of measurement errors on \hat{k} . The transient experiment is assumed to be run from $t = 0$ to $T = 0.6$ with measurements made only at the outlet of the

reactor ($S=1$) with the dimensionless length $x = 0.12$. In addition, only measurements of temperature will be made. Results for $R = 30$, $N = 12$, $k^0 = 15$, $\gamma = 2 \times 10^3$, $\sigma = 0.1, 0.3$ and 0.5 are shown in Table II-6. Steepest descent appears to be more sensitive to the level of errors as σ increases. Computing times for the results in Table II-6 are approximately 20 seconds for steepest descent and 40 seconds for quasilinearization.

Table II-6. Effect of the Level of Measurement Error on \hat{k} (Transient Case, Temperature Measurements Only)

σ		Steepest Descent	Quasilinearization
0.1	\hat{k}	30.26595	30.27132
	iterations	5	4
	% error	0.35	0.37
0.3	\hat{k}	29.92751	30.48781
	iterations	5	4
	% error	0.77	1.10
0.5	\hat{k}	34.05261	29.77492
	iterations	8	4
	% error	12.98	1.20

The effect of R for $S = 1$, $N = 12$, $k^0 = 15$, $\gamma = 8 \times 10^3$, $\sigma = 0.3$ is shown in Table II-7. As R decreases, the error increases, both methods yielding almost identical results. Again quasilinearization takes roughly twice as long as steepest descent. It is now

interesting to see whether the errors can be decreased significantly by also measuring the concentration at the reactor outlet. We consider the case then $S = 1$ with $R = 10$, $N = 12$, $\sigma = 0.3$, in comparison with the $R = 10$ case in Table II-7. When both variables are measured $\hat{k} = 30.74994$ (1.97% error) and 30.68687 (1.75% error) for steepest descent and quasi-linearization, respectively.

Table II-7. Effect of Number of Measurement Times R on \hat{k} (Transient Case, Temperature Measurements Only)

R		Steepest Descent	Quasilinearization
30	\hat{k}	30.48145	30.48781
	iterations	5	4
	% error	1.07	1.10
15	\hat{k}	29.58272	29.58610
	iterations	7	4
	% error	1.92	1.91
10	\hat{k}	31.49580	31.53761
	iterations	9	4
	% error	4.46	4.60

5.3 Example 3: Estimation of Petroleum Reservoir Permeabilities

The pressure behavior of a reservoir in the vicinity of a single producing well can be described by a radial form of the heat equation in which there are two concentric regions of different permeabilities, an inner region and an outer region [59]. A technique for determining

reservoir properties in the vicinity of a well is a drillstem test in which the reservoir pressure at the well is measured during a period of constant production followed by a shut-in period. If $u_1(x,t)$ and $u_2(x,t)$ represent the pressures in the inner and outer regions, respectively, where x is the distance from the wellbore, the transient pressure behavior is governed by

$$u_{1t} = \frac{k_1}{\alpha} e^{-2\lambda x} u_{1xx} \quad 0 < x < x_a \quad (76)$$

$$u_{2t} = \frac{k_2}{\alpha} e^{-2\lambda x} u_{2xx} \quad x_a < x < 1 \quad (77)$$

$$u_1(x,0) = u_2(x,0) = p_0 \quad (78)$$

$$u_{1x} = \frac{\beta}{k_1} q(t) \quad x = 0 \quad (79)$$

$$u_{2x} = 0 \quad x = 1 \quad (80)$$

$$u_1(x_a, t) = u_2(x_a, t) \quad (81)$$

$$k_1 u_{1x} = k_2 u_{2x} \quad x = x_a$$

$$q(t) = \begin{cases} 100 \text{ bbl/day} & 0 \leq t \leq t_f \\ 0 & T \geq t \geq t_f \end{cases} \quad (82)$$

The problem is to estimate the two permeabilities k_1 and k_2 from measurements of the well pressure,

$$y(0, t_r) = u_1(0, t_r) + (\text{errors}) \quad r = 1, 2, \dots, R \quad (83)$$

We employ the following parameter values: $\alpha = 0.00289$ darcy-min, $\lambda = 10.074$, $x_a = 0.36$, $p_o = 400$ psi, $\beta = 36.35$ psi--darcy/cu.ft/min, $t_f = 100$ min and $T = 200$ min. The true values of k_1 and k_2 are both assumed to be 10 md. As before, the noisy observations are generated by

$$y(0, t_r) = u_1^*(0, t_r) [1 + \sigma \text{Gauss}(0, b)] \quad (84)$$

where u_1^* is the solution of (76)-(82) with $k_1 = k_2 = 10$ md.

The results of steepest descent are presented in Table II-8. Even in the case of no measurement errors, both k_1 and k_2 are estimated relatively inaccurately. With one percent error, the k_2 estimate deteriorates considerably. Since the only measurement is at the $x = 0$ boundary, it is necessary to observe the response as long as possible to ascertain the effect of k_2 on $u_1(0, t)$.

Table II-8. Results of Estimation of Permeabilities by Steepest Descent

σ	b	R	Initial Guess		\hat{k}_1	\hat{k}_2	Iterations	Time (sec)
			k_1	k_2				
0	0	20	15.0	15.0	10.284	9.608	10	160
0.1	0.1	200	15.0	15.0	9.748	11.293	7	114

5.4 Conclusions

The following conclusions can be drawn from the computational results:

(1) Steepest descent is slightly more sensitive to the level of experimental error than is quasilinearization; however, both methods are generally effective at levels approaching 15% error.

(2) Steepest descent is roughly 1.5 to 2.0 times as fast as quasilinearization for the specific computations reported. This comparison will depend in general on k^0 , γ , and N .

(3) The range of initial guesses for which convergence can be obtained for the steepest descent method is larger than that of the quasilinearization.

(4) The quasilinearization converges faster than the method of steepest descent and the quasilinearization exhibits quadratic convergence, if convergent at all. The choice of the step length γ is important for the rate of convergence in steepest descent. If γ is chosen arbitrarily, numerical experiments are necessary to determine the range of γ values necessary for convergence. Otherwise, γ can be computed from the second variation of J at the expense of the additional computing required.

(5) In the first two examples highly accurate estimates were obtained with measurements at only a few spatial locations. A possible conclusion is that better estimates can be obtained by taking data for as long a time as possible at a few locations rather than at many locations for a short time. However, this question is very much dependent

on the initial condition $u_0(x)$ and the shape of $u(x,t)$ and may not be true in general.

(6) Estimates of k in the plug flow reactor were improved markedly by measuring both concentration and temperature at the reactor outlet as opposed to temperature only. The general strategy of measuring as many state variables as possible has also been shown for ordinary differential equations [68].

(7) A confidence interval analysis can be used to select the best estimate from a group of estimates. In addition, computation of H represents a necessary condition for observability, which depends in general on n , m , p , R , and S as well as on the location of the S measurements. The optimal location of S measurements can be determined by minimizing the variances of the parameter estimates. The results show the advantage of using the observations taken at the optimal measurement locations to estimate the parameters.

(8) The trial-function expansion is not only a desirable method for solving partial differential equations but also a useful tool for parameter estimation because it could considerably simplify and shorten the computational effort involved in determining the parameters in complicated systems.

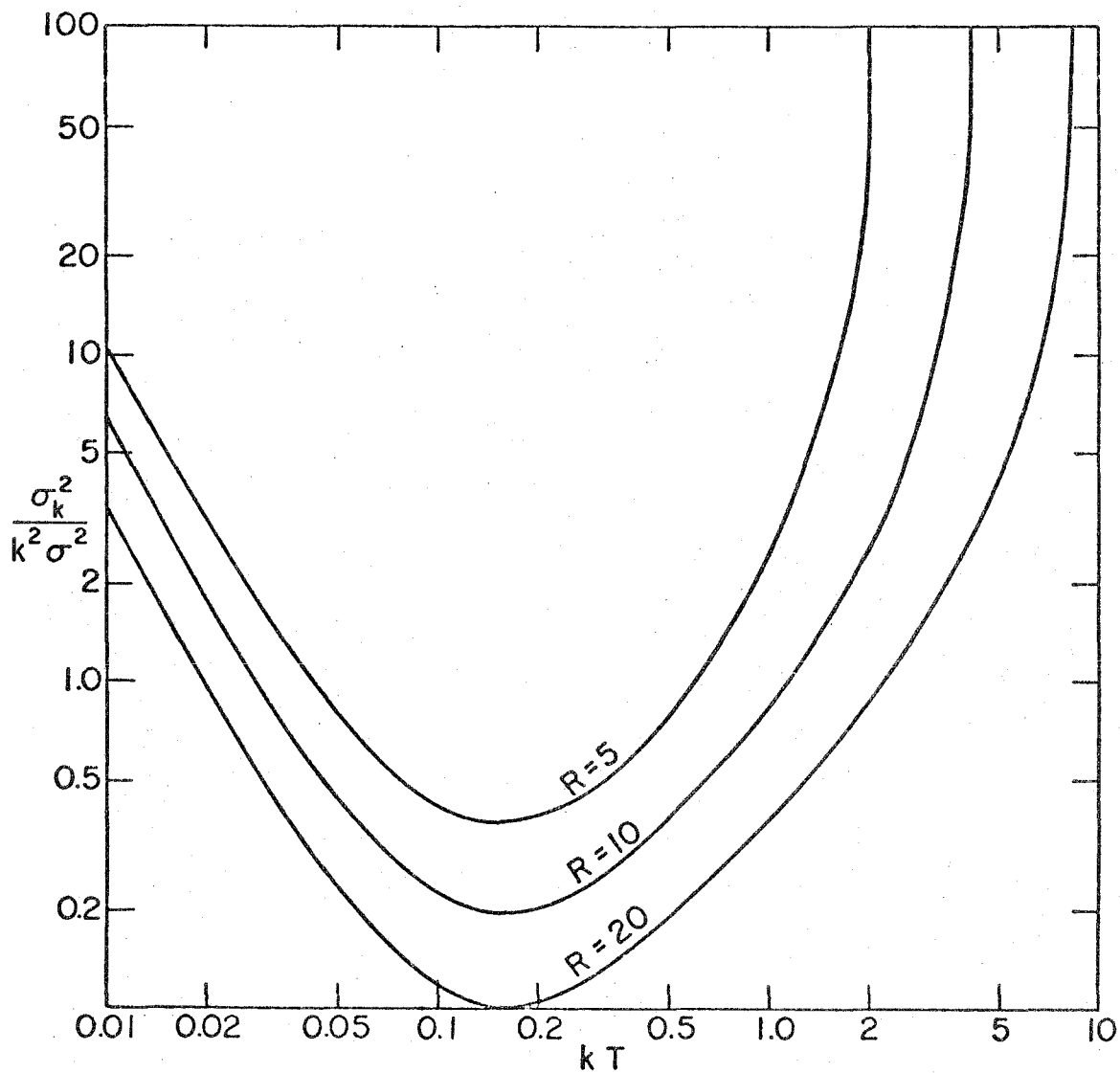


Figure II-1: Dimensionless variance of parameter estimate in heat equation for various values of kT

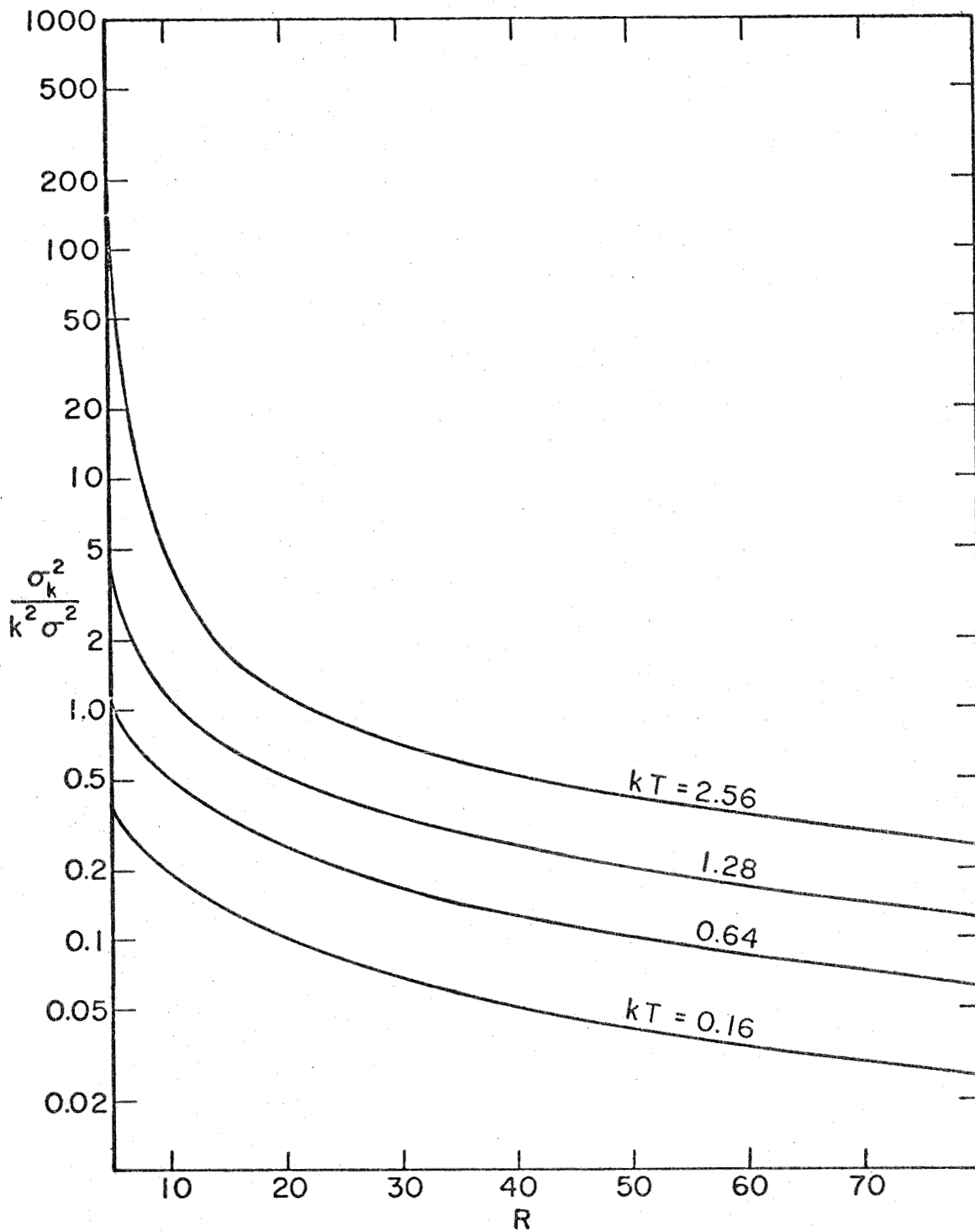


Figure II-2. Dimensionless variance of parameter estimate in heat equation for various values of R .

Appendix II-A

ANALYSIS OF THE GENERATION OF EXPERIMENTAL ERRORS

The value of k estimated by any technique will be a random variable because it is based on a particular set of experimental errors generated on the computer. Although in different computer experiments errors were generated with the same mean and standard deviation, different sample values were generated. In order to examine the distribution of estimated values, 50 sets of data were used to estimate k in (46) by steepest descent with $k^0 = 0.5$, $S = 9$, $R = 20$, $T = 0.2$, $a = 0$, $b = 0.3$, $\sigma = 0.3$ and $\gamma = 0.5$. This distribution of \hat{k} values obtained is shown in Figure II-3.

Since every \hat{k} is a function of the sample values, each \hat{k} is a random variable. If we assume the 50 values of \hat{k} are samples from a normal distribution with mean μ and variance σ_e^2 , we can estimate μ and σ_e^2 from these 50 values. Let \tilde{k} denote the mean value of \hat{k} from the 50 samples, and let $\hat{S}^2 = \frac{1}{49} \sum_{i=1}^{50} (\hat{k}_i - \tilde{k})^2$. Then the variable $7(\tilde{k} - \mu) / \hat{S}$ obeys the Student's distribution. In this set of \hat{k} , $\tilde{k} = 1.0132$ and $\hat{S} = 0.967 \times 10^{-2}$. For a 90% confidence level, the true value of μ can be expected to lie between

$$1.0109 < \mu < 1.0155$$

We note, of course, that μ will not necessarily be equal to k^* and from this set of 50 estimates it appears very unlikely that for a very large number of experiments μ does equal k^* .

We can use the exact confidence interval analysis presented earlier for $\hat{k} = 1.0132$, from which we obtain a standard deviation of 1.22×10^{-2} . This is reasonable agreement with the value computed from the experiments in Figure II-A.1. Note that in the calculation of the standard deviation the variance of the errors of data is approximated by

$$\sigma^2 = \frac{1}{n-1} \sum_{r=1}^R \sum_{s=1}^S [y_{r,s} - u(t_r, x_s, \hat{k})]^2 \quad (\text{II-A.1})$$

where n is the number of experimental data.

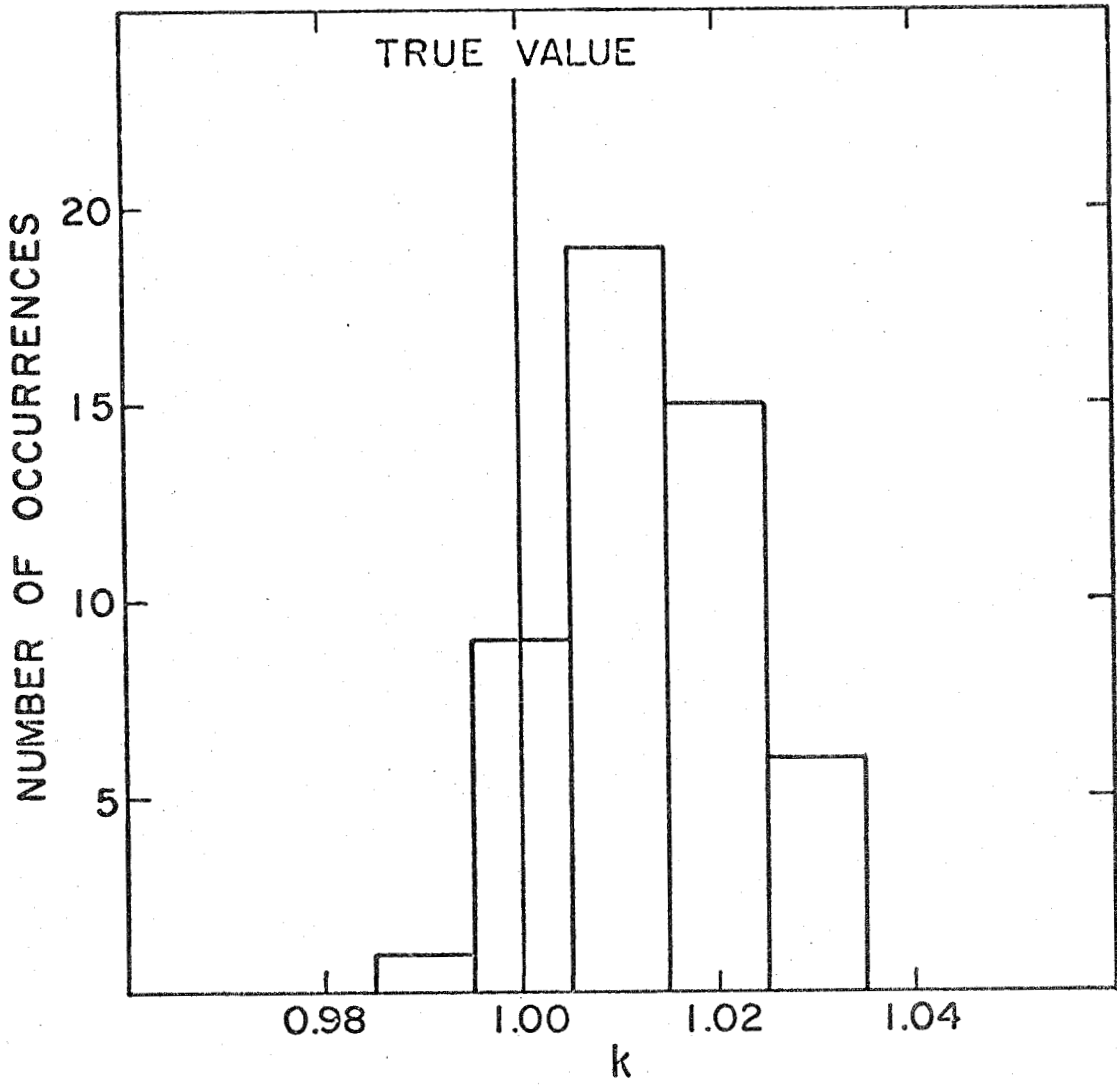


Figure II-A-1: Number of occurrences of k from 50 experiments

Appendix II-B

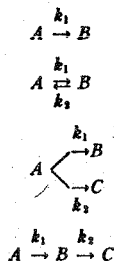
The Accuracy of Kinetic Parameters Estimated from Batch and Integral Reactor Data

A. L. RAVIMOHAN, W. H. CIEN and J. H. SEINFELD

Department of Chemical Engineering, California Institute of Technology, Pasadena, California 91109, U.S.A.

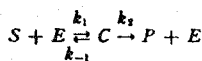
The accuracy of rate constant estimates obtained by minimizing the sum of squares of differences between observed and calculated concentrations is considered. Closed solutions are obtained for some basic types of first order reaction schemes. The results are presented in the form of plots of the dimensionless variance of parameter estimates. The kineticist can use the plots both in analyzing experiments and in planning them for maximum economy. Such advance studies are capable of providing valuable insight into questions of experimental design even when the reaction scheme is unknown.

The estimation of rate constants from experimental concentration-time measurements in batch and tubular flow reactors is an important problem in chemical engineering. Two steps are involved in the overall problem. First, estimates of the rate constants must be obtained. It is now recognized that the correct procedure that must be used is least squares analysis of the measured data. Since, for experimental reasons, the measured quantities are usually the concentrations, the least squares criterion must be applied to the raw concentration vs. time data. This step can be conveniently carried out using quasilinearization^(1,2,3). It is the object of this paper to consider the second step, namely the analysis of the accuracy of kinetic parameter estimates, for the four reaction schemes:



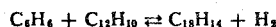
It is shown that in addition to this type of post-facto analysis, the results can also be used for the systematic planning of kinetic experiments.

Rosenbrock and Storey⁽⁴⁾ present a general technique for the determination of confidence intervals for parameter estimates in ordinary differential equations. Heineken, *et al.*⁽⁵⁾ used this procedure to determine confidence intervals for parameter estimates in the enzymatic reactions



Seinfeld and Gavalas⁽⁶⁾ used quasilinearization to estimate the rate constants and Rosenbrock and Storey's procedure to analyze the estimates in the pyrolytic dehydrogenation of benzene to diphenyl and triphenyl,

On a étudié l'exactitude des estimés relatifs à la constante de vitesse qu'on obtient en minimisant la somme des carrés des différences entre les concentrations observées et celles qu'on a calculées. On obtient des solutions fermées pour certains genres fondamentaux de systèmes de réaction de premier ordre. On présente, sous forme de graphiques, les résultats de la variance sans dimensions des estimés des paramètres. Le préposé à la cinétique peut utiliser les dits graphiques pour analyser le travail expérimental et le planifier pour minimiser son coût. Des études préliminaires de ce genre permettent d'obtenir une connaissance précieuse des questions relatives à la conception de travaux expérimentaux, lorsqu'on ne connaît pas le système de réaction.



The present work represents a continuation of the effort to provide experimental kineticists with easily-interpretable results on the accuracy of rate constant estimates in common reactions.

The general problem may be stated as one of estimating the parameters in a set of ordinary differential Equations⁽⁴⁾. The state of a system is governed by the set of ordinary differential Equations

$$\dot{x}_i = f_i(x, a, t) \quad i = 1, 2, \dots, n \quad x_i(t_0) = x_{i0} \dots (1)$$

which contain p unknown parameters, a_i , $k = 1, 2, \dots, p$. Experimental observations z_j , $j = 1, 2, \dots, m$, are made at R values of t , t_1, t_2, \dots, t_R , and are known functions of the system state, $g_j(x)$, but contain additive random experimental errors η_j ,

$$(z_j)_r = g_j[x(t_r)] + (\eta_j)_r \quad j = 1, 2, \dots, m; r = 1, 2, \dots, R \dots (2)$$

The error vectors n , corresponding to different sets of measurements are assumed to be statistically independent. The errors in the individual elements of each vector n , are assumed to be normally distributed with zero mean and covariance matrix M_r . The parameters a are estimated to minimize the weighted sum of squares

$$S^2 = \sum_{r=1}^R [z_r - g(x(a, t_r))]^T M_r^{-1} [z_r - g(x(a, t_r))] \dots (3)$$

where $x(a, t)$ is the solution of Equation (1), with known initial conditions.

We present only the formulas required to compute confidence intervals. If the experimental error variances are small enough for linearization to be valid, the error in the parameter estimates obtained by minimizing S^2 will be normally distributed with zero mean and covariance matrix P . If the initial conditions x_0 are known without error

$$P = H^{-1} \dots (4)$$

Reprinted in Canada from
 THE CANADIAN JOURNAL OF CHEMICAL ENGINEERING
 Vol. 48: 420-427: August 1970
 A Publication of The Chemical Institute of Canada
 151 Slater Street, No. 906, Ottawa 4, Ontario

where

$$H = \sum_{i=1}^n D_i^T G_i^T M_i^{-1} G_i D_i \dots (5)$$

and

$$\begin{aligned} \dot{D} &= AD + B \\ D(t_0) &= 0 \end{aligned} \dots (6)$$

$$\begin{aligned} A &= \{A_{ij}\} = \left(\frac{\partial f_i}{\partial x_j} \right)_{a^*} \\ B &= \{B_{ij}\} = \left(\frac{\partial f_i}{\partial a_j} \right)_{a^*} \dots (7) \\ G &= \{G_{ij}\} = \left(\frac{\partial g_i}{\partial x_j} \right)_{a^*} \end{aligned}$$

a^* being the value of a minimizing S^2 . Heineken, *et al.*⁽⁶⁾ show that as $R \rightarrow \infty$ the matrix H defined in Equation (5) rapidly approaches

$$Rk = \frac{R}{T - t_0} \int_{t_0}^T D(t)^T G(t)^T M(t)^{-1} G(t) D(t) dt \dots (8)$$

The variance of any linear combination of the a for an arbitrary vector b is $\sigma_a^2 = b^T P b$. Complete details are given by Rosenbrock and Storey⁽⁶⁾.

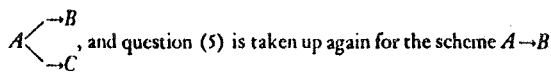
In the analysis to follow we make the assumptions:

1. The initial concentrations are known without error.
2. The initial charge in each case consists of pure A .
3. The concentrations are measured directly.
4. Unless otherwise indicated, the covariance matrix of experimental errors, $M(t)$ has the simple form $\sigma^2 I$.

We examine the effect of the following on the confidence intervals of the rate constant estimates:

1. How many data points R should be taken and over what range in order to attain a given accuracy of parameter estimates.
2. What effect does the level of experimental error have on the problem.
3. Above what value of R can Equation (8) be taken as an adequate representation of Equation (5).
4. How many of the n independent concentrations should be measured, and which ones chosen in the event of a choice being available.
5. What advantage can be gained by measuring more than the independent number of concentrations.
6. Instead of spacing the observation points equally in the time interval (t_0, T) , might it not be advantageous to space the same number of points in a different manner. In particular, what is the effect of spacing them equally in the conversion interval $(1, \xi)$ rather than the corresponding time interval (t_0, T) .
7. If concentration-time data from runs at different temperatures are used to determine the rate constants and activation energies, how accurate would these estimates be. At how many temperatures should observations be taken in order to achieve a given accuracy.

Questions (1) and (2) are answered for all the four reaction schemes. (3) is considered for the schemes $A \rightleftharpoons B$ and $A \rightarrow B \rightarrow C$. (4) and (5) are thoroughly discussed for the scheme



where the matrix of experimental errors $M(t)$ has a form different from the $\sigma^2 I$ usually assumed. The simple scheme $A \rightarrow B$ is also used to illustrate how the same techniques can be used to answer the more complicated questions (6) and (7).

Results

Following Heineken *et al.*, dimensionless parameters of the type $\psi_i = \frac{\sigma_i^2 R}{k_i^2 \sigma^2}$ were used to correlate the results. Here, k

is the mean value and σ_i^2 the variance of an estimated parameter, R the number of data points, and σ^2 the variance of the dimensionless forms of the experimentally measured concentrations. The ψ_i are obtained as diagonal elements of the matrix $PR/\sigma^2 k^2$, where $P = H^{-1}/R$ for large R and $P = H^{-1}$ in general. The ψ_i parameter contains information regarding the

accuracy of an estimate (the larger the value of $\frac{k^2}{\sigma_i^2}$, the more

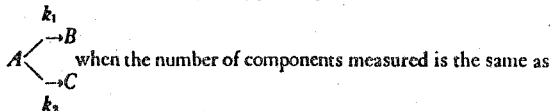
accurate is the estimate), for any given value of the experimental error. It also incorporates the number of observations R , and can be used to decide what value of R is necessary in order to get an acceptable accuracy of the estimate. Plots of ψ_i are therefore a concise and convenient representation of the results of the study. They can be used to plan kinetic experiments which seek to obtain accurate estimates of parameters when approximate values are known from a less sophisticated analysis.

Figure 1 presents $\psi_1 = \frac{\sigma_{k_1}^2 R}{k_1^2 \sigma^2}$ and $\psi_2 = \frac{\sigma_{k_2}^2 R}{k_2^2 \sigma^2}$ versus $k_1 T$

for the isothermal scheme $A \rightleftharpoons B$. The curve of $\psi_1 = \frac{\sigma_{k_1}^2 R}{k_1^2 \sigma^2}$

for the scheme $A \rightarrow B$ is also shown for comparison. Figures

2 and 3 show the same type of plots for $A \rightarrow B \rightarrow C$ and



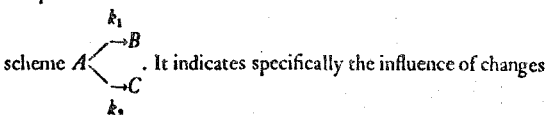
the number of independent components = 2, and these are chosen to be A and B .

Figure 4 illustrates some typical results when the exact formula $P = H^{-1}$ is used for computation instead of the approxi-

mation $P = H^{-1}/R$ in the isothermal scheme $A \rightleftharpoons B$. Similar

curves for $A \rightarrow B \rightarrow C$ are shown in Figure 5. Figure 6 is a cross-plot of Figure 5 in which the asymptotic approach to the approximate formula as R increases is clearly seen.

Figure 7 is an attempt to answer the question of how many components and which ones should be measured in the isothermal



in the G matrix on the accuracy of estimation, and D matrix remaining the same and the M matrix continuing to be $\sigma^2 I$. This important question is raised again for the isothermal scheme $A \xrightarrow{k_1} B$, but this time the G matrix is kept constant at col [1 - 1]. The source of variation now is the matrix of experimental errors M . M is taken to be $\begin{pmatrix} \sigma_A^2 & 0 \\ 0 & \sigma_B^2 \end{pmatrix}$, which represents independent measurements on A and B with different variances. This, of course, is a more realistic assumption than $M = \sigma^2 I$. $s = \frac{\sigma_A}{\sigma_B}$ is allowed to vary, and the results are shown in Figure 8.

In Figure 9, the effect of unequal division of the time interval is explored for the isothermal scheme $A \rightarrow B$. When the time interval (t_0, T) is equally divided by R points, it can be shown that

$$\psi_1 = \frac{\sigma_{k_1}^2 R}{k_1^2 \sigma_A^2} = \frac{R}{\sum_1^R (k_1 t_r) \exp(-2k_1 t_r)} \dots (9)$$

where

$$t_r = t_0 + \frac{r(T-t_0)}{R} \quad r = 1, \dots, R.$$

When the conversion interval $(1, \xi)$ is equally divided by R points, the corresponding result is

$$\psi_1 = \frac{\sigma_{k_1}^2 R}{k_1^2 \sigma_A^2} = \frac{R}{\sum_1^R (x_r \ln x_r)^2} \dots (10)$$

where

$$x_r = 1 - \frac{r(1-\xi)}{R} \quad r = 1, \dots, R$$

and

$$\xi = \exp\{-k_1(T-t_0)\}$$

As R becomes large, Equations (5) and (8) should converge to the same value.

In Figure 10, the dimensionless variances of the frequency factor and activation energy estimates are plotted against the number of temperatures at which observations are taken.

$$\psi_G = \frac{\sigma_G^2 R}{G^2 \sigma^2} = \frac{h_{22}}{G^2 \sigma^2 |h|}$$

$$\psi_E = \frac{\sigma_E^2 R}{E^2 \sigma^2} = \frac{h_{11}}{E^2 \sigma^2 |h|}$$

where

$$h = \sum_{l=0}^L \left\{ \frac{1}{\sigma^2(T-t_0)} \int_{t_0}^T \begin{bmatrix} D_1^2 & D_1 D_2 \\ D_1 D_2 & D_2^2 \end{bmatrix} dt \right\} \dots (11)$$

It must be noted that Equation (11) represents a hybrid expression which is h from the point of view of each run but is actually

H from the point of view of $\sum_{l=0}^L$. Hence, $P = h^{-1}/R$ and no

division by L is necessary. Very large values of L are experimentally unrealistic as the number of temperatures at which isothermal runs are conducted seldom exceeds 10.

Discussion of results

The discussion of each figure appears below the figure.

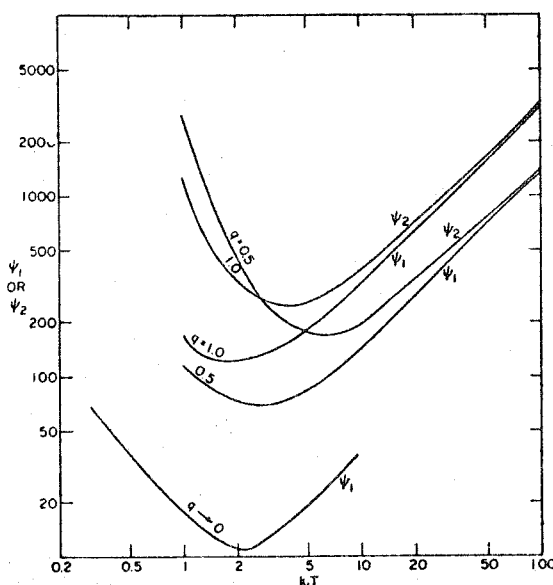


Figure 1—Dimensionless variance of parameter estimates vs. dimensionless time in the reaction scheme $A \xrightleftharpoons[k_2]{k_1} B$, when only component A is measured and the number of observations R is large.

Fig. 1

For each value of $q = \frac{k_2}{k_1}$ there exists a minimum value of

ψ_1 and ψ_2 corresponding to a particular $k_1 T$. As q decreases, the value of $k_1 T$ at which the minimum occurs at first increases. This is because as k_2/k_1 decreases, more B is present at equilibrium and it takes longer for the reaction to achieve equilibrium. In order to obtain maximum accuracy it is necessary in this case to continue taking measurements for a longer time. However,

when $\frac{k_2}{k_1}$ becomes very small, the amount of A present at equilibrium tends to zero. Due to the error in measuring A , there is not much point in taking a large number of observations when its concentration is very low. Hence the optimum value of $k_1 T$ starts decreasing as $\frac{k_2}{k_1}$ approaches 0.

For small values of $k_1 T$, k_1 can be estimated more accurately than k_2 . In this range, the smaller the value of q , the greater the accuracy that can be obtained in ψ_1 . Conversely, in this range, the smaller the value of q , the lesser the accuracy that can be obtained in ψ_2 . This is because the smaller the value of q the more significant is the forward reaction. If, on the other hand, measurements are continued for a long time (high $k_1 T$), this difference gets narrowed down. This is because more of the observations are now being taken close to equilibrium and are effectively being wasted.

Fig. 2

For small values of $k_1 T$ (small extent of reaction) the dimensionless variance ψ_1 tends to zero, because only the first step in the reaction is important and k_1 can be estimated accurately by a large number of measurements carried out over the interval $(0, T)$. As q increases, the rate of the second reaction relative to the first increases and ψ_1 increases for small values of $k_1 T$. This is because it becomes harder to estimate k_1 from observations over the fixed interval $(0, T)$ due to the increasing effect of the second reaction.

For small values of $k_1 T$, ψ_2 increases rapidly because of the inability to observe the effect of the second reaction which is

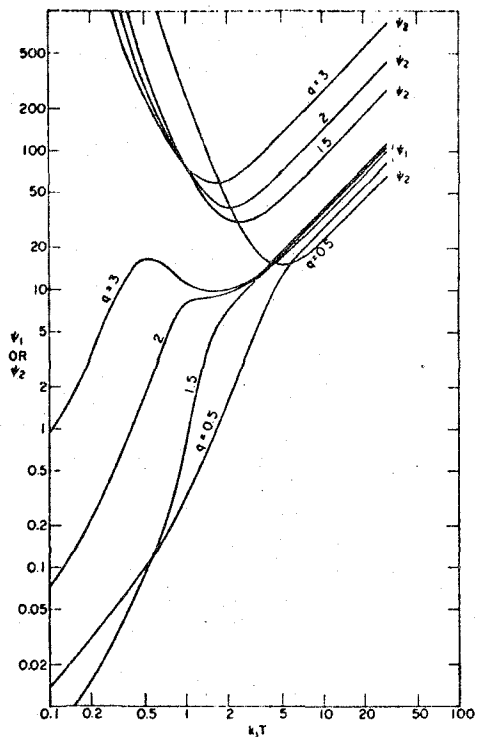


Figure 2—Dimensionless variance of parameter estimates vs. dimensionless time in the reaction scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$, when components A and B are measured and the number of observations R is large.

necessary to estimate k_2 . Conversely, ψ_1 , for small $k_1 T$, as q increases, ψ_2 decreases, because the second reaction becomes important.

For large values of $k_1 T$, both ψ_1 and ψ_2 increase with $k_1 T$, the more accurate estimates corresponding to smaller values of q . Smaller values of q correspond to a longer time necessary for complete conversion to C and the ability to obtain more information on a fixed interval $(0, T)$. As a result, the ψ_2 curves exhibit a minimum coupled with a reversal of the dependence on q . For $q = 3$ the ψ_1 curve also exhibits a minimum (a relative minimum) reflecting the trade-off between the increase in ψ_1 at high values of $k_1 T$, the decrease in ψ_1 at low values of $k_1 T$ and the effect of a large k_2/k_1 which causes an increase in ψ_1 for moderate values of $k_1 T$.

Fig. 3 For very small and very large values of $k_1 T$ both ψ_1 and ψ_2 become large. In the former case it is because neither reaction has proceeded to any appreciable extent. In the latter case, the low accuracy is due to the fact that most of the measurements are being wasted in measuring values of A and B which have, for all practical purposes, long since reached their final values. The trade-off between these two considerations results in a minimum

in both the ψ_1 and ψ_2 curves for all values of $q = \frac{k_2}{k_1}$.

As q increases, the value of $k_1 T$ corresponding to the minimum value of the ψ_1 and ψ_2 curves decreases. This is a direct consequence of measurements being taken on A and B only. The higher the value of q for a given k_1 , the more important the second reaction becomes. It is then advantageous to take

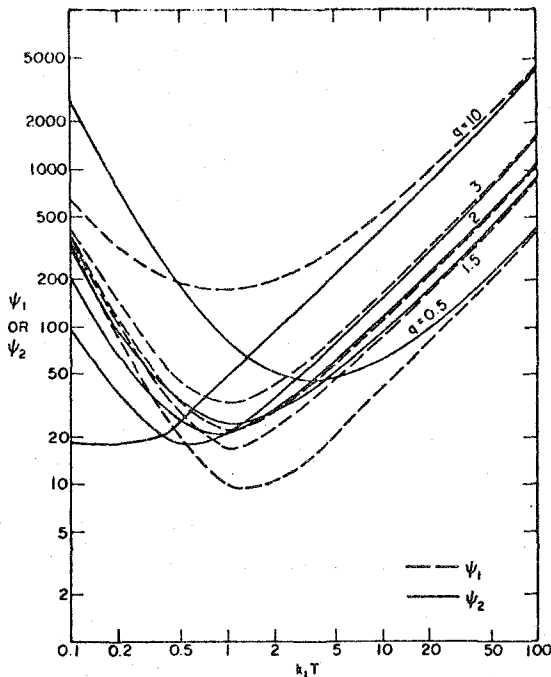


Figure 3—Dimensionless variance of parameter estimates vs. dimensionless time in the reaction scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ when components A and B are measured and the number of observations is large.

measurements on A and B before all the A is converted to C by the second reaction and the value of B becomes static. The optimum value of $k_1 T$ therefore becomes smaller as q increases.

For values of q less than about 2, ψ_1 is less than ψ_2 , i.e. k_1 is estimated more accurately than k_2 . But for higher values of q , the situation is exactly the opposite. This effect is important for low values of $k_1 T$, and is again a consequence of the fact that we are observing only A and B. We may think of the measurements on A as determining $(k_1 + k_2)$ and the measurements on B as determining k_1 . As q increases, it becomes less and less profitable to measure B as the predominant reaction is the second one. Hence the k_1 estimates start getting less and less accurate. However, under these circumstances, $(k_1 + k_2)$ becomes very nearly the same as k_2 itself, and therefore the accuracy of the k_2 estimate does not suffer as much. For low values of q , on the other hand, the situation is exactly the opposite; k_2 estimates are poor because we are effectively taking no observations on the second reaction.

Fig. 4 In general, as R is increased the accuracy of the estimates of k_1 and k_2 is increased.

For small values of $k_1 T$, smaller values of ψ_1 and ψ_2 are obtained with fewer measurements. This is because ψ_1 and ψ_2 depend on the product of σ_i^2 and R, and as R decreases, the decrease in R more than compensates for the increase in σ_i^2 . For large values of $k_1 T$, as R decreases, σ_i^2 increases faster than R decreases and ψ_1 and ψ_2 increase. At large values of $k_1 T$, ψ_1 and ψ_2 depend very strongly on R, and it is in this range that R should be made as large as possible.

Fig. 5 For small values of $k_1 T$ and $R = 5, 10, 20$, ψ_1 and ψ_2 are not strongly dependent on R. If $R = \infty$, a significant decrease in ψ_1 and ψ_2 occurs. For large values of $k_1 T$, ψ_1 and ψ_2 are strong functions of R. Thus, if the reaction is allowed to proceed

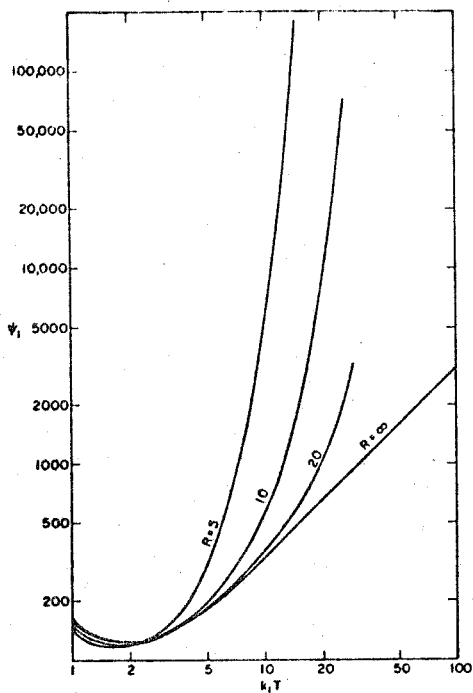


Figure 4—Effect of number of observations R on the dimensionless variance of k_1 estimate vs. dimensionless time in the reaction scheme $A \rightleftharpoons B$ when only component A is measured and $q = \frac{k_2}{k_1} = 1$.

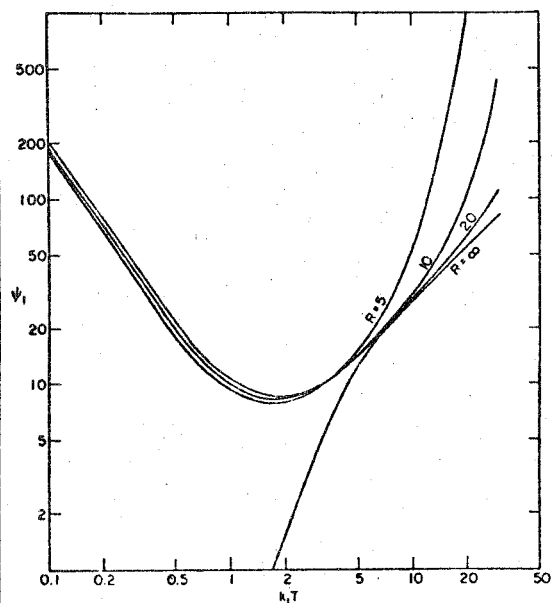


Figure 5—Effect of number of observations R on the dimensionless variance of k_1 estimate vs. dimensionless time in the reaction scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$, when components A and B are measured and $q = \frac{k_2}{k_1} = 0.5$.

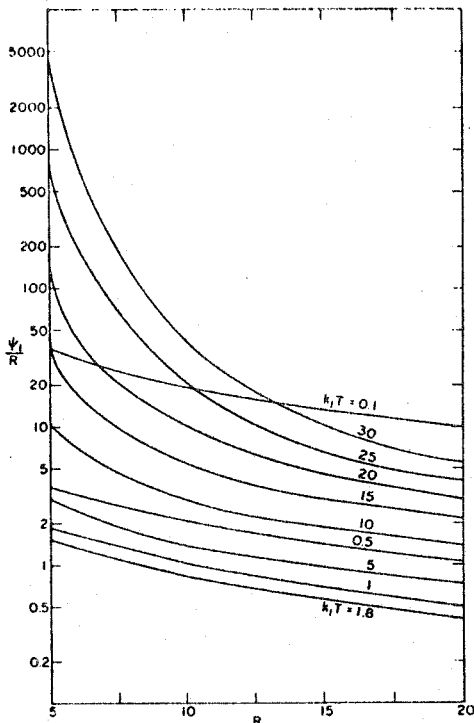


Figure 6—Effect of number of observations R on the accuracy of k_1 estimate in the reaction scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$, when components A and B are measured and $q = \frac{k_2}{k_1} = 0.5$ (cross-plot of Figure 5).

substantially toward the complete conversion to C, it is important for a fixed value of T that one make as many measurements as possible. If the reaction is stopped early, then the number of observations is not as important. These conclusions are clearly visible in Figure 6 in which $\frac{\psi_1}{R}$ is plotted against R for constant values of k_1T .

Fig. 7 The number of independent components in a reaction scheme must be equal to the number of independent reactions. Also, they must be chosen in such a way that the stoichiometric matrix A relating them to the extents of the independent reactions be non-singular.

$$\begin{pmatrix} C_1 \\ \vdots \\ C_a \end{pmatrix} = A \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix}$$

In many problems of kinetic parameter estimation, there is a choice regarding which components are to be measured. Seinfeld and Gavalas⁽⁶⁾ come to the conclusion that one should try and measure as many of the R independent concentrations as possible; and that if a choice must be made, intermediates give better parameter estimates than primary constituents.

In the present study, this question was thoroughly examined

for the isothermal scheme $A \begin{cases} \xrightarrow{k_1} B \\ \xrightarrow{k_2} C \end{cases}$. Figure 7 is an example of the

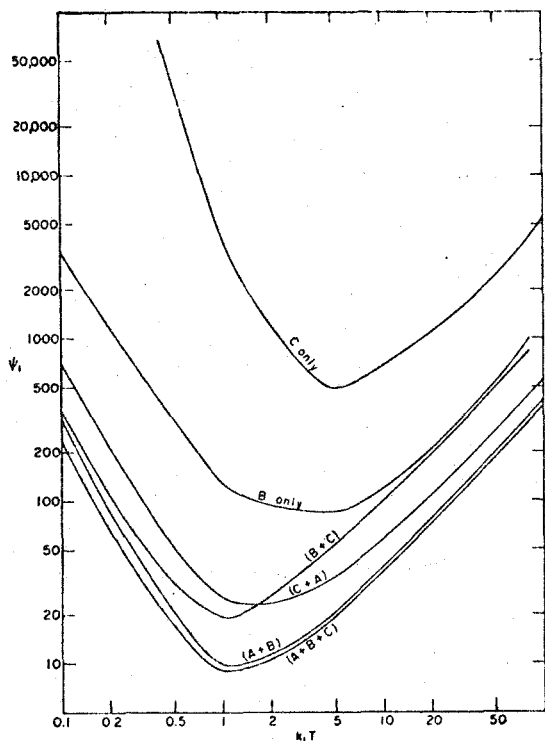


Figure 7—Effect of number of components measured on the dimensionless variance of k_1 estimate vs. dimensionless

time in the reaction scheme $A \begin{cases} \xrightarrow{k_1} B \\ \xrightarrow{k_2} C \end{cases}$, when the number of observations R is large and $q = \frac{k_2}{k_1} = 0.5$.

large number of plots that were obtained for various values of $\frac{k_2}{k_1}$. The only conclusion that is valid for all these plots is that the most accurate estimates of k_1 and k_2 are obtained when all the three components are measured. However, a certain combination of two components always comes very close to the $(A + B + C)$ curve. Hence it would appear that there is little advantage in measuring more than the independent number of concentrations when the error matrix M has the form $\sigma^2 I$.

For specific guidance in an actual problem, it is necessary to look at the plot for the relevant value of $\frac{k_2}{k_1}$. Consider, for example, $\frac{k_2}{k_1} = 0.5$ which is illustrated in Figure 7. Further, let us confine our attention to the ψ_1 curves which give information regarding the accuracy of the k_1 estimate. Here, the best two components to measure are obviously A and B . Measuring C and A is better for high values of $k_1 T$, but B and C is better for lower values of $k_1 T$. Near the optimum values of $k_1 T$, there is little to choose between these two combinations.

The best single component to measure is B . Measurement of C alone is likely to lead to extremely inaccurate estimates. Of course, measurement of A and C is better for lower values of $k_1 T$, there is little to choose between these two combinations.

The best single component to measure is B . Measurement of C alone is likely to lead to extremely inaccurate estimates. Of course, measurement of A and C is better for lower values of $k_1 T$, there is little to choose between these two combinations.

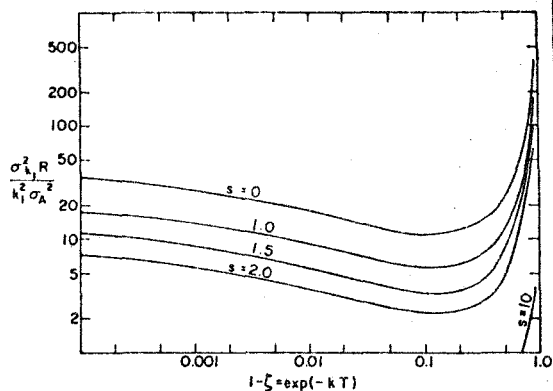


Figure 8—Effect of measuring more than the number of independent components on the dimensionless variance of parameter estimate vs. conversion in the reaction scheme

$A \rightarrow B$ when the covariance matrix of errors is $M = \begin{pmatrix} \sigma_A^2 & 0 \\ 0 & \sigma_B^2 \end{pmatrix}$

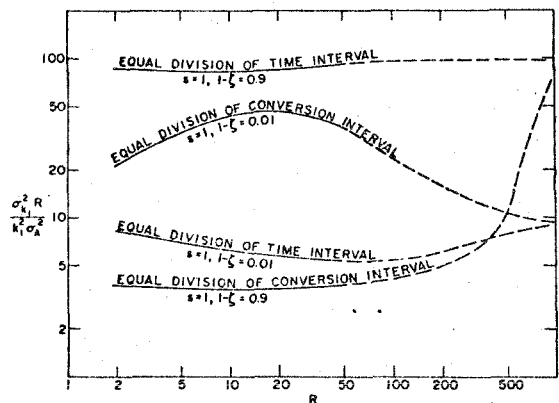


Figure 9—Effect of distribution of experimental observations on the dimensionless variance of parameter estimate vs. number of observations in the reaction scheme $A \rightarrow B$.

The existence of H^{-1} is an essential requirement in the procedure of Rosenbrock and Storey⁽⁴⁾. Evidence from the present work confirms that the non-singularity of H is a sufficient condition for the estimability of parameters in a system of first order linear ordinary differential equations.

Fig. 8 For a given σ_A and a given number of observations R , the accuracy of estimation improves as s increases. This is correct as increasing s means increasing accuracy of measuring B . The curve for $s = 0$ corresponds to extremely imprecise measurements on B , which is equivalent to measurement of A alone.

Measuring more than the number of independent components is advantageous under all circumstances except $s = 0$. Further, for every value of n , there is a minimum which represents the point at which the reaction must be skipped to get maximum accuracy of estimate.

As $T \rightarrow t_0$ ($\xi \rightarrow 1$), all the curves go up to infinity. This is obvious as there can be no estimates when the reaction is not carried out at all.

Fig. 9 The limiting value plotted in Figure 9 is strictly valid for a very large number of observations. This limit is approached

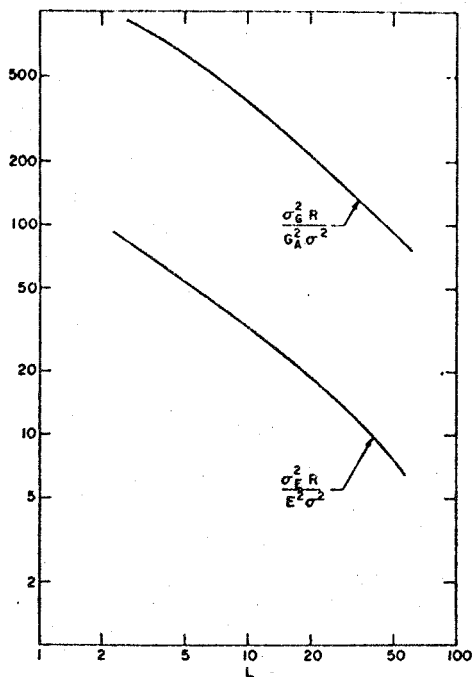


Figure 10—Effect of number of isothermal runs on the dimensionless variances of the frequency factor and activation energy estimates in the scheme $A \xrightarrow{G_A \exp(-E/\theta)} B$

with $G_A T = 10$, $\frac{\theta(0)}{E} = \frac{1}{5}$, $\frac{\theta(L)}{E} = \frac{1}{3}$

rapidly from the lower side when the time interval (t_0, T) is equally divided. However, if the same number of observations are taken at intervals of equal conversion, the results are profoundly different. For high values of ξ (e.g. 0.9), it is possible to achieve much greater accuracies by this device. For low values of ξ (e.g. 10^{-3}), on the other hand, this must not be done as errors increase greatly. In fact, for low ξ , the limit as $R \rightarrow \infty$ is approached from the upper side. We therefore conclude that taking a finite number of observations at equal conversion intervals will be useful when the reaction has to be stopped far from completion. The physical meaning of this is that when concentrations are changing rapidly, observations must be taken more frequently, but when they are changing slowly, the time period between observations can be lengthened. The experimental kineticist very often makes use of this trick while collecting his data.

Fig. 10 The accuracy of estimation of G_A and E improves almost in direct proportion to the number of temperatures at which observations are taken.

In the limited range considered, the activation energy is estimated more accurately than the frequency factor. This would indicate that non-linear regression of the pooled data yields a better estimate of E than that obtained by regressing the estimated rate constants at different temperatures. In such cases, the technique presented in this paper could be invaluable in assigning confidence limits to the parameters obtained by the non-linear analysis.

Conclusion

The statistical structure of several basic first order reaction schemes was analyzed. No analysis of experimental kinetic data is complete without a good estimate of the accuracy of the rate constants derived therefrom. The first use of the present results is in obtaining such estimates for any desired confidence

level from the computed variance of the rate constant error distribution. The second and more important use is in planning experiments to obtain maximum kinetic information without sacrifice of accuracy. Questions such as how many data points to take and in what range, which components should be measured in the event of a choice being available, and what effect the level of experimental errors has on the problem, were answered. The same technique was also extended to answer some novel questions such as how to distribute the observations in a given time interval, and at how many temperatures isothermal runs must be conducted to get acceptable estimates of the frequency factor and activation energy. The practising chemical engineer should find the procedure extremely useful even when confronted by reaction schemes more complex than the ones considered here. Even if this type of complete analysis is not undertaken, the simple first order schemes should give him a feel for the effects of features like reversibility, parallelism and consecutiveness in the reaction mechanism on the propagation of error.

Acknowledgment

This work was supported by the U.S. Atomic Energy Commission under Project Agreement No. 1 under AT(04-3)-767 and a Chevron Oil Field Research Company Grant.

APPENDIX: THE WORKING EQUATIONS

We will illustrate the details of the analysis for the scheme



Under the assumptions in the introduction, the reaction is described by

$$\frac{dx_1}{dt} = -(k_1 + k_2) x_1; x_1(0) = 1$$

$$\frac{dx_2}{dt} = k_1 x_1; x_2(0) = 0$$

where $x_1 = [A]/[A_0]$ and $x_2 = [B]/[A_0]$ and A and B have been chosen as the independent components. Therefore,

$$x_1 = \exp[-(k_1 + k_2)t]$$

$$x_2 = \frac{k_1}{k_1 + k_2} [1 - \exp\{-(k_1 + k_2)t\}]$$

In this case, $n = 2$, $p = 2$ and D is a 2×2 matrix governed by

$$\frac{dD_{11}}{dt} = -(k_1 + k_2) D_{11} - x_1; D_{11}(0) = 0$$

$$\frac{dD_{12}}{dt} = -(k_1 + k_2) D_{12} - x_1; D_{12}(0) = 0$$

$$\frac{dD_{21}}{dt} = k_1 D_{11} + x_1; D_{21}(0) = 0$$

$$\frac{dD_{22}}{dt} = k_1 D_{12}; D_{22}(0) = 0$$

The integrated forms are

$$D_{11} = -t \exp[-(k_1 + k_2)t]$$

$$D_{12} = -t \exp[-(k_1 + k_2)t]$$

$$D_{21} = \frac{k_1 t}{k_1 + k_2} \exp[-(k_1 + k_2)t] - \frac{k_2}{(k_1 + k_2)^2} [\exp\{-(k_1 + k_2)t\} - 1]$$

$$D_{22} = \frac{k_1 t}{k_1 + k_2} \exp[-(k_1 + k_2)t] + \frac{k_1}{(k_1 + k_2)^2} [\exp\{-(k_1 + k_2)t\} - 1]$$

When, for example, only A is measured, $G = [1 \ 0]$, and

$$D^T G^T G D = \begin{bmatrix} D_{11}^2 & D_{11} D_{12} \\ D_{12} D_{11} & D_{12}^2 \end{bmatrix}$$

h is now easily obtained from Equation (8). The results of other cases are summarized below.

Isothermal case

a) $A \xrightarrow{k_1} B$. $n = 1, p = 1$

$$D = -t \exp(-k_1 t)$$

b) $A \xrightarrow[k_2]{k_1} B$. $n = 1, p = 2$

$$D_1 = -\frac{k_2}{(k_1 + k_2)^2} - \frac{k_1}{(k_1 + k_2)^2} t \exp\{-(k_1 + k_2)t\} + \frac{k_2}{(k_1 + k_2)^2} \exp\{-(k_1 + k_2)t\}$$

$$D_2 = \frac{k_1}{(k_1 + k_2)^2} - \frac{k_1}{k_1 + k_2} t \exp\{-(k_1 + k_2)t\} - \frac{k_1}{(k_1 + k_2)^2} \exp\{-(k_1 + k_2)t\}$$

c) $A \xrightarrow[k_2]{k_1} B \rightarrow C$. $n = 2, p = 2$

$$D_{11} = -t \exp(-k_1 t)$$

$$D_{12} = 0$$

$$D_{21} = \frac{k_1}{k_1 - k_2} t \exp(-k_1 t) + \frac{k_2}{(k_1 - k_2)^2} \exp(-k_1 t) - \frac{k_2}{(k_1 - k_2)^2} \exp\{-k_2 t\}$$

$$D_{22} = -\frac{k_1}{k_1 - k_2} t \exp(-k_2 t) + \frac{k_1}{(k_1 - k_2)^2} \exp(-k_2 t) - \frac{k_1}{(k_1 - k_2)^2} \exp(-k_1 t)$$

Isothermal runs at different temperatures

If $A \rightarrow B$ and $k_1 = G_A \exp(-E/\theta)$ we will consider the l^{th} experiment with temperature θ_l . Since $n = 1$ and $p = 2$ (G_A and E), D is given by

$$D_1 = -t \exp[-t G_A \exp(-E/\theta_l) - E/\theta_l]$$

$$D_2 = \frac{t G_A}{\theta_l} \exp\left[-t G_A \exp\left(-\frac{E}{\theta_l}\right) - \frac{E}{\theta_l}\right]$$

Nomenclature

a	= p -dimensional parameter vector
b	= arbitrary p -dimensional vector
c	= n -dimensional initial value vector
A, B, C, E, P, S	= components in various reactions
D	= $n \times p$ matrix
E	= activation energy divided by the gas constant
f	= n -dimensional vector function
g	= m -dimensional known function of state variables
G	= $m \times n$ matrix
G_A	= frequency factor
h	= $p \times p$ matrices
H	
k_1, k_2	= rate constants
L	= number of equal divisions of temperature interval
M	= covariance matrix of experimental error
n	= number of independent components
p	= number of parameters to be estimated
P	= covariance matrix of parameter estimates
q	= k_2/k_1
R	= number of equal divisions of the time interval
S^2	= sum of squares being minimized
s	= σ_A/σ_B
t	= time variable
t_0	= lower limit of time interval
T	= upper limit of time interval
x	= n -dimensional state vector
z	= m -dimensional vector of observations
ζ	= extent of an independent reaction
η	= random additive experimental error
θ	= absolute temperature
ξ	= lower limit of conversion interval
$\sigma_A^2, \sigma_B^2, \sigma^2$	= variances of experimental error
$\sigma_{k_1}^2, \sigma_{k_2}^2, \sigma_G^2, \sigma_E^2$	= variances of parameter estimates
ψ_1, ψ_2	= dimensionless variances of parameter estimates

References

- (1) Bellman, R. and Kalaba, R., "Quasilinearization and Nonlinear Boundary Value Problems", American Elsevier, New York (1965).
- (2) Donnelly, J. K. and Quon, D., AIChE Tampa Meeting, Paper 19f, May 19-22 (1968).
- (3) Lee, E. S., Ind. Eng. Chem. Fundamentals, 7, No. 1, 152 (1968).
- (4) Rosenbrock, H. H. and Storey, C., "Computational Techniques for Chemical Engineers", Pergamon, New York (1966).
- (5) Heincken, F. G., Tsuchiya, H. M. and Aris, R., Math. Biosciences, 1, 115 (1967).
- (6) Seinfeld, J. H. and Gavalas, G. R., "Analysis of Kinetic Parameters from Batch and Integral Reaction Experiments", AIChE Journal, 16, 4, 644 (1970).

Manuscript received May 27, 1969; accepted March 24, 1970.

★ ★ ★

Appendix II-C

SOCIETY OF PETROLEUM ENGINEERS OF AIME
6200 North Central Expressway
Dallas, Texas 75206

PAPER
NUMBER SPE 4282

THIS IS A PREPRINT — SUBJECT TO CORRECTION

Reliability of Reservoir Parameters from History Matched Drill Stem Tests

By

Thomas N. Dixon, Member AIME, U. of Texas at Austin;
John H. Seinfeld, California Institute of Technology;
Richard A. Startzman, Member AIME, Chevron Oil Field Research Co.; and
W. H. Chen, California Institute of Technology

© Copyright 1973
American Institute of Mining, Metallurgical, and Petroleum Engineers, Inc.

This paper was prepared for the Third Numerical Simulation of Reservoir Performance Symposium of the Society of Petroleum Engineers of AIME to be held in Houston, Tex., Jan. 10-12, 1973. Permission to copy is restricted to an abstract of not more than 300 words. Illustrations may not be copies. The abstract should contain conspicuous acknowledgment of where and by whom the paper is presented. Publication elsewhere after publication in the JOURNAL OF PETROLEUM TECHNOLOGY or the SOCIETY OF PETROLEUM ENGINEERS JOURNAL is usually granted upon request to the Editor of the appropriate journal provided agreement to give proper credit is made.

Discussion of this paper is invited. Three copies of any discussion should be sent to the Society of Petroleum Engineers office. Such discussion may be presented at the above meeting and, with the paper, may be considered for publication in one of the two SPE magazines.

ABSTRACT

An important use of simulation is to determine reservoir properties by interpreting transient well tests. In general, this determination is carried out by systematically varying reservoir properties until the pressures computed by the simulator match pressures measured during the well test - a procedure known as history matching. Reservoir properties determined by history matching are subject to error. Here we present a method of estimating this error. As an example, we studied the problem of estimating porosity and permeability in both a homogeneous reservoir and one in which damage is present in the vicinity of the well. Results presented indicate that the accuracy of calculated reservoir parameters depends on (1) the type of parameter estimated, (2) the number of parameters estimated, (3) the true value of the parameters and (4) the design of the well test.

INTRODUCTION

Research efforts in history-matching reservoir simulators have principally been directed toward improving and extending existing techniques with respect to decreasing computing time. Little attention has been paid, however, illustrations at end of paper.

to the analysis of the accuracy of the parameter values from the history match. Without such an analysis, parameter estimates from history matching might be meaningless. The problem is to estimate errors in parameter values determined by history matching.

The theory that is presented in the Appendix is applicable in general to multiphase, two-dimensional simulators. However, as an illustration, we apply the theory to the well known radial form of the diffusion equation,

$$\frac{\partial (kr \frac{\partial p}{\partial r})}{r \partial r} = \phi \mu c \frac{\partial p}{\partial t} \dots \dots \dots (1)$$

describing the transient behavior of pressure in a radial, horizontal reservoir containing a single-phase fluid of small and constant compressibility. The equation allows for permeabilities to change with radial distance from a wellbore - a situation that might be encountered if damage is present. We assume that the reservoir is finite. Furthermore, we assume that the well produces at a constant rate for a certain time and then is shut in. Thus, both drawdown and buildup takes place. No wellbore storage effects are considered.

The history-matching procedure that is

generally used to find the permeability, k , and the porosity, ϕ , in a reservoir is as follows.

1. Make an initial guess of k and ϕ .
2. Run the simulator with these values of k and ϕ .
3. Compare well pressures computed by the simulators to those measured in the well.
4. If these pressures do not match, change the parameters k and ϕ and make repeated runs until an acceptable match is obtained.

In this report we are not concerned with the procedure used to obtain a match, but are concerned with errors associated with the parameters obtained by history matching. A parameter is any quantity that is both (1) unknown and (2) affects the behavior of the mathematical model. A parameter can be some readily identifiable physical quantity, such as permeability or porosity. It can also be more abstract, such as the rate of change of permeability with radial distance from a wellbore.

If θ_1^{true} is the true, but unknown value of Parameter 1 and θ_1^{est} is its value that has been estimated by some history-matching process, then the error can be defined as

$$\Delta\theta_1 (\text{error}) = \theta_1^{true} - \theta_1^{est} \dots (2)$$

We can never determine the exact error in estimating any particular parameter, but we can compute statistical properties that give us a measure of the error. A statistical property of importance is the standard deviation of the error, σ_θ . A large standard deviation would indicate that the estimated value for that parameter is probably not accurate. The mathematical procedure used to compute standard deviations is given in the Appendix.

APPLICATION TO DRILLSTEM TESTS

We now present the results of the application of the theory in the Appendix to determining the reliability of parameters estimated from history-matched drillstem tests. We assume that the reservoir behavior is described by Eq. 1.

In order to generalize our results, we considered the dimensionless parameters defined below:

$$\phi (\text{"porosity"}) =$$

$$256.68 \frac{\phi hc \ln \left(\frac{r_e}{r_w} \right) r_w^2 p_e}{t_t q B} \dots (3)$$

$$K(x) (\text{"permeability"}) = 1.1215 \times 10^{-3} \frac{hp_e}{\mu \ln \left(\frac{r_e}{r_w} \right) q B} \cdot k(x), \dots (4)$$

where all symbols except t_t and x are standard SPE symbols. We assume that the well test is a fairly simple one, namely, one flow period followed by one shut-in period. The total test period in days is t_t . The spatial variable, x , is the dimensionless distance from the wellbore defined as $\ln(r/r_w)/\ln(r_e/r_w)$. $K(x)$ can be a function of distance from the wellbore. In the homogeneous case, $K(x)$ is a constant.

Using the dimensionless time $\tau = t/t_t$ and dimensionless pressure $p^* = p/p_i$, the reservoir model is

$$\frac{\partial p^*}{\partial t} = \frac{\exp(-2 \ln(r_e/r_w)x)}{\phi} \frac{\partial}{\partial x} \left[K(x) \frac{\partial p^*}{\partial x} \right] \dots (5)$$

$$p^*(x, 0) = 1 \quad 0 \leq x \leq 1 \dots (6)$$

$$\frac{\partial p^*}{\partial x} \Big|_{x=0} = \frac{1}{2\pi K(0)} \quad 0 \leq \tau \leq t_f \dots (7)$$

$$\frac{\partial p^*}{\partial x} \Big|_{x=0} = 0 \quad t_f < \tau \leq 1 \dots (8)$$

$$\frac{\partial p^*}{\partial x} \Big|_{x=1} = 0 \quad 0 \leq \tau \leq 1, \dots (9)$$

where t_f is the fraction of the total test time during which flow takes place.

Case 1 - Homogeneous Reservoir
(K and ϕ Constant)

In this case we considered either K or ϕ or both to be unknown and computed standard deviations of the errors in each parameter.

Numerical experiments revealed that these standard deviations varied, depending on which parameters were being estimated, the values of the parameters, the number of parameters estimated, and the design of the well test. In Figs. 1 and 2 we show the results of cases in which either porosity only or permeability only are determined by history matching. All other parameters are assumed to be known.

Determining Φ Only

A measure of the error in Φ is the function, ψ_Φ . Where

$$\psi_\Phi = \frac{\sigma_\Phi}{\Phi \sigma_p} \dots \dots \dots (10)$$

σ_Φ is the standard deviation of the error in Φ , and σ_p is the standard deviation of the well pressure measurements. In Fig. 1 we show ψ_Φ as a function of dimensionless permeability for a given value of Φ . Also shown is ψ_Φ for two different values of t_f . t_f is the ratio of the flow period to the total test period (flow plus buildup). From Fig. 1 we can see that ψ_Φ increases with K . This means that the accuracy with which porosity can be determined decreases with increased permeability. For a given value of K , however, ψ_Φ decreases with increased t_f . This indicates that porosity can best be determined if the flow portion of the test is as long as possible ($t_f = 1.0$).

Determining K Only

A measure of the error in K is the function, ψ_K . Where

$$\psi_K = \frac{\sigma_K}{K \sigma_p} \dots \dots \dots (11)$$

σ_K is the standard deviation of the error in K . Fig. 2 shows ψ_K as a function of dimensionless permeability for each of two different constant values of porosity and two different values of t_f . ψ_K can be seen to increase with permeability in all cases. Thus, the accuracy with which permeability can be determined decreases with increased values of permeability. Fig. 2 also shows that smaller values of porosity improve the accuracy with which permeability can be estimated by history matching. In addition, Fig. 2 shows that larger values of t_f result in better estimates of permeability.

Determining Both Φ and K

In Figs. 3 through 5, we show the results of cases in which both porosity and permeability are simultaneously determined by history matching. All other parameters are assumed to be known. Figs. 3 and 4, when compared to Figs. 1 and 2, show that each parameter is determined

with less accuracy than if only one is to be determined.

The dependence of ψ_Φ and ψ_K on t_f is not as straightforward as in the above cases in which only one parameter is to be determined. Fig. 5 shows that ψ_Φ and ψ_K actually pass through minima at $t_f \sim 0.65$. This indicates that, under the specific conditions outlined in Fig. 5, namely that $K = 4.45 \times 10^{-3}$ and $\Phi = 6.45 \times 10^{-7}$, the optimum well test design would be to flow the well approximately 65 percent of the total test time. For this flow time, parameter accuracy would be maximum.

Case 2 - Permeability Varies With Distance From Wellbore

In this case we considered a situation in which permeability varied with distance from the wellbore. The dependence of permeability on distance was assumed to be

$$K(x) = K_1 + K_2 x \dots \dots \dots (12)$$

K_1 is the permeability at the wellbore. K_2 is the rate of change of permeability with distance. A positive value of K_2 would indicate that permeability is increasing away from the wellbore.

Fig. 6 represents the case when both K_1 and K_2 are to be estimated by history matching. All other parameters are assumed to be known. ψ_{K_1} and ψ_{K_2} are shown as functions of K_1 . If σ_{K_1} and σ_{K_2} are the standard deviations of K_1 and K_2 , respectively, and σ_p is the standard deviation of the pressure measurements, then

$$\psi_{K_1} = \frac{\sigma_{K_1}}{K_1 \sigma_p} \dots \dots \dots (13)$$

and

$$\psi_{K_2} = \frac{\sigma_{K_2}}{K_2 \sigma_p} \dots \dots \dots (14)$$

The standard deviations of both parameters in Fig. 6 increase with K_1 . Also, both ψ_{K_1} and ψ_{K_2} are lower when permeability is decreasing with distance from the wellbore ($K_2 = -K_1$) than when permeability is increasing ($K_2 = +K_1$). This latter observation indicates that, in the situation studied, the dependence of permeability on distance from the wellbore (Eq. 12) can be best determined when permeability decreases away from the wellbore.

Fig. 7 shows ψ_{K_1} and ψ_{K_2} as functions of t_f for fixed values of K_1 and K_2 . As in the

case of estimating both Φ and K in the homogeneous reservoir, minima occur, indicating optimum test shut-in times for minimizing standard deviations in the estimated parameters.

Case 3 - Two-Region Permeability

Another ideal situation studied was one in which the reservoir is represented by two concentric regions of different permeabilities. We assumed that these permeabilities were the only parameters to be estimated and that the boundary location, x^* , between the two regions was known.

The two permeabilities are denoted by K_i (internal) and K_e (external). The variables considered are (1) the ratio of K_i to K_e ($\beta = K_i/K_e$) and (2) the fraction, t_f , of the time during which the well flows.

Fig. 8 shows ψ_{K_i} and ψ_{K_e} vs K_i for $\beta = 0.1, 1$ and 10 and $\Phi = 6.47 \times 10^{-4}$, $t_f = \frac{1}{2}$ and $x^* = 0.36$. As K_i decreases, both ψ_{K_i} and ψ_{K_e} decrease significantly; that is, the decreases in σ_{K_i} and σ_{K_e} are more than enough to compensate for the decrease in K_i . There is very little effect of β on ψ_{K_i} . However, β has a much stronger effect on ψ_{K_e} . At large values of K_i it appears that both ψ_{K_i} and ψ_{K_e} go through a maximum, indicating that the rate of increase of σ_{K_e} decreases as K_i increases. Clearly, the estimates of K_i and K_e will be more accurate if both K_i and K_e are small and will improve as β increases.

Fig. 9 shows ψ_{K_i} and ψ_{K_e} vs the flow fraction of the total test for $\beta = 0.1, 1$ and 10 . Fig. 9 could be used to design single well tests, since the time at which the well is shut in can be controlled in the test. Although the effect of the variation in shut-in time is not dramatic, we note that better estimates of K_i and K_e can be obtained if the production period is extended as long as possible. Again, significantly better estimates of K_e can be obtained if β is large, and the value of β is much more important in the estimation of K_e than in K_i .

CONCLUSIONS

A method has been developed to obtain standard deviations for reservoir parameters estimated from history matching. The studies presented indicate that the accuracy of calculated reservoir parameters depends on the following points.

1. The type of parameter estimated. Some

parameters can evidently be determined with more accuracy than others.

2. The number of parameters estimated. The greater the number of parameters estimated, the greater the error in determining the value of each.

3. The true values of the parameters. In some cases, errors in estimating parameters were found to be functions of the actual value of the parameters.

4. The design of the well test. Errors in the values of porosity and permeability were shown to be functions of the relative times of shut-in and buildup periods in a drillstem test.

Point 4 indicates that the analysis presented is useful in designing optimum drillstem tests to determine reservoir properties with optimum accuracy.

APPENDIX

Petroleum reservoirs are commonly modeled using a set of partial differential equations derived from conservation laws. Unless we have perfect knowledge regarding the rock and fluid properties of the reservoir system of interest, these equations contain unknown parameters. Typical examples of these parameters are permeability and porosity.

In this section we will present the methods used in this study to compute standard deviations of reservoir parameters determined from history-matched drillstem tests. These methods are also applicable to large-scale simulation models. However, the computing time necessary to compute standard deviations of parameters for large-scale systems may be excessive.

Consider a function $p_i(\theta)$. p represents wellbore pressure, θ represents a set of parameters ($\theta_j, j=1, 2, \dots, N$) and i is an index representing points in time. For the sake of illustration let us consider a case in which only one parameter, the j^{th} parameter, has been estimated by some history-matching process. If θ_j^{est} is the estimated value of the parameter and θ_j^{true} is the true, but unknown, value of the parameter, then define an error, $\Delta\theta_j$, as follows.

$$\Delta\theta_j = \theta_j^{\text{true}} - \theta_j^{\text{est}} \dots \dots \dots (A-1)$$

p_i^{obs} is the observed pressure at the i^{th} time. It is a function of the true, but unknown, value of the j^{th} parameter so that

$$\begin{aligned}
 p_i^{obs} &= p_i(\theta_j^{true}) \\
 &= p_i(\theta_j^{est} + \Delta\theta_j) \dots (A-2)
 \end{aligned}$$

Let us now represent the function p_i ($\theta_j^{est} + \Delta\theta_j$) by a first-order Taylor's series. We have assumed here that the history match is sufficiently close ($\Delta\theta$ small) so that the higher order Taylor series terms are essentially zero.

$$\begin{aligned}
 p_i(\theta_j^{est} + \Delta\theta_j) &= \\
 p_i(\theta_j^{est}) + \lambda_{ij} \cdot \Delta\theta_j, \dots (A-3)
 \end{aligned}$$

where λ_{ij} is a "sensitivity coefficient" defined as

$$\begin{aligned}
 \lambda_{ij} &= \frac{\partial p_i}{\partial \theta_j} \text{ evaluated at } \theta_j = \theta_j^{est}. \\
 \dots \dots \dots (A-4)
 \end{aligned}$$

If we have M observations of pressure, p_i^{obs} ($i=1, 2, \dots, M$), then we can obtain an estimate of the parameter, θ_j , from the following formula.

$$\sigma_{\theta_j}^2 = \frac{\sigma_p^2}{\sum_{i=1}^m \lambda_{ij}^2} =$$

variance of parameter θ_j (A-5)

Eq. A-5 was obtained by taking the variance of both sides of the least-squares estimate of $\Delta\theta$ from Eq. A-3. It was assumed that the λ_{ij} are known exactly and that the variance of the error in the observed wellbore pressures, σ_p^2 , is constant and does not vary with time.

If the errors in the observed wellbore pressures are normally distributed with a mean error of zero and a standard deviation of $\sigma_p = \sqrt{\sigma_p^2}$, then we can place statistical confidence limits on the true value of the j th parameter. Thus, there is a $1-\alpha$ probability that the true θ_j^{true} falls within a certain range:

$$\begin{aligned}
 \theta_j^{est} - \frac{\sigma_p^{t_{m-1, \alpha/2}}}{\left(\sum_i \lambda_{ij}^2\right)^{1/2}} \leq \theta_j^{true} \leq \theta_j^{est} \\
 + \frac{\sigma_p^{t_{m-1, \alpha/2}}}{\left(\sum_i \lambda_{ij}^2\right)^{1/2}}, \dots (A-6)
 \end{aligned}$$

where $t_{m-1, \alpha/2}$ is the t-statistic for $m-1$ degrees of freedom and $(1-\alpha)$ confidence limits.

Similar reasoning can be used in the case where there are two or more parameters to be estimated. Eq. A-3 now becomes

$$\begin{aligned}
 p_i(\theta^{est} + \Delta\theta) &= \\
 p_i(\theta^{est}) + \sum_{j=1}^N \lambda_{ij} \Delta\theta_j, \dots (A-7)
 \end{aligned}$$

where the θ 's now represent the set of all parameters ($\theta_j, j=1, 2, \dots, N$). The $\sigma_{\theta_j}^2$'s are elements of the main diagonals of the symmetric matrix C, where

$$\begin{aligned}
 C = \begin{bmatrix} \sigma_{\theta_1}^2 & \dots & \dots & \dots & \sigma_{\theta_1 \theta_2}^2 \\ \vdots & \sigma_{\theta_2}^2 & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ \sigma_{\theta_1 \theta_2}^2 & & & & \sigma_{\theta_M}^2 \end{bmatrix} \\
 \dots \dots \dots (A-8)
 \end{aligned}$$

The diagonal elements are the variances of each parameter and the off-diagonal elements are covariances. We did not make use of the covariances in this study. They serve primarily to indicate the amount of correlation between the parameters and do not affect our conclusions.

The matrix C is computed from the sensitivity coefficients λ_{ij} by

$$C = (\Lambda^T \Lambda)^{-1} \sigma_p^2, \dots (A-9)$$

where

$$\Lambda = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \dots & \dots & \lambda_{1N} \\ \vdots & \lambda_{22} & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & \ddots & \vdots \\ \lambda_{M1} & & & & \lambda_{MN} \end{bmatrix}$$

In the foregoing analysis it was assumed that the sensitivity coefficients λ_{ij} were available. There are two ways to compute λ 's.

Finite Differences

Here the λ 's are computed by (for one parameter)

$$\lambda_{ij} = \frac{p_i(\theta_j^{est} + \delta\theta_j) - p_i(\theta_j^{est})}{\delta\theta_j} \dots \dots \dots (A-10)$$

Sensitivity Equations

In this case, the sensitivity coefficients are determined from solutions to a partial differential equation for λ_j . This equation is derived from the original mathematical model represented by Eq. 1. If we differentiate both sides of Eq. 1 with respect to θ_j , we can obtain an equation that has λ_j as a dependent variable instead of p . The sensitivity coefficient λ_{ij} (λ_j evaluated at time, i) can be found. In this study, sensitivity coefficients were obtained from numerical solutions of these sensitivity equations.

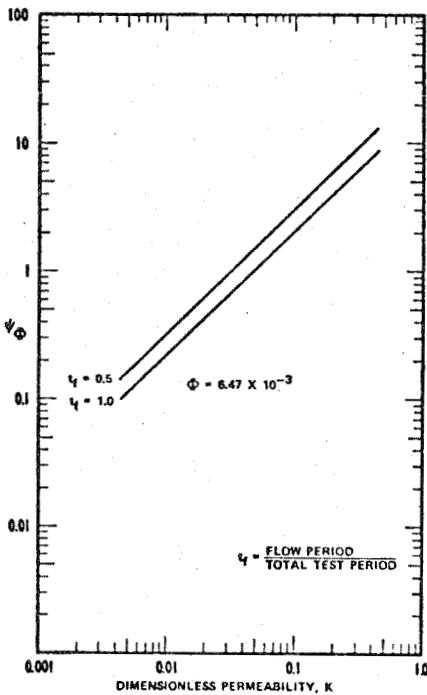


Fig. 1 - λ_ϕ as a function of dimensionless permeability. Homogeneous reservoir. Estimation of only ϕ .

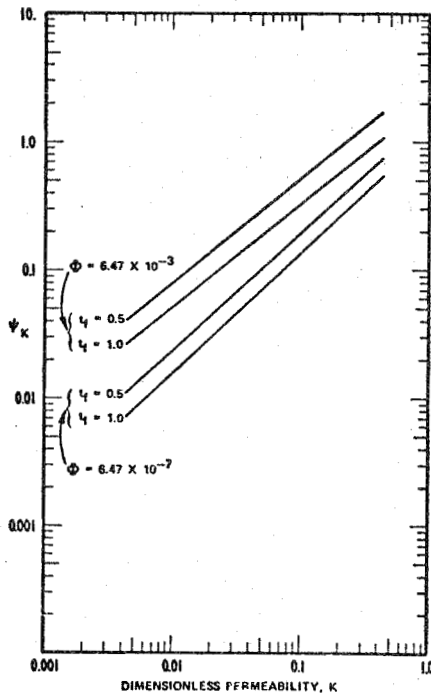


Fig. 2 - λ_K as a function of dimensionless permeability. Homogeneous reservoir. Estimation of only K .

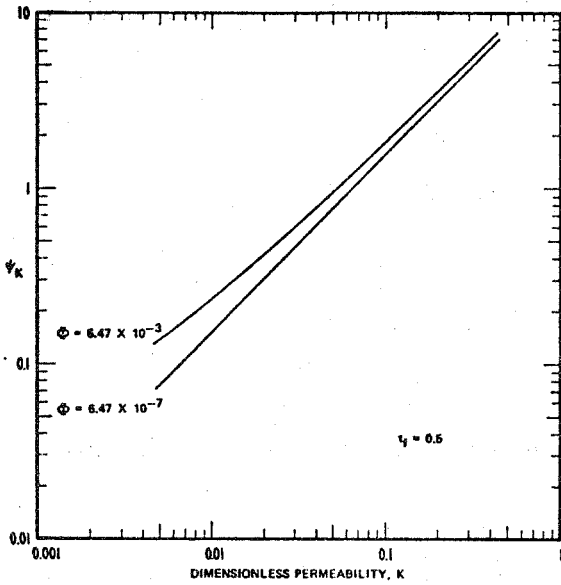


Fig. 3 - ψ_K as a function of dimensionless permeability. Homogeneous reservoir. Estimation of both K and ϕ .

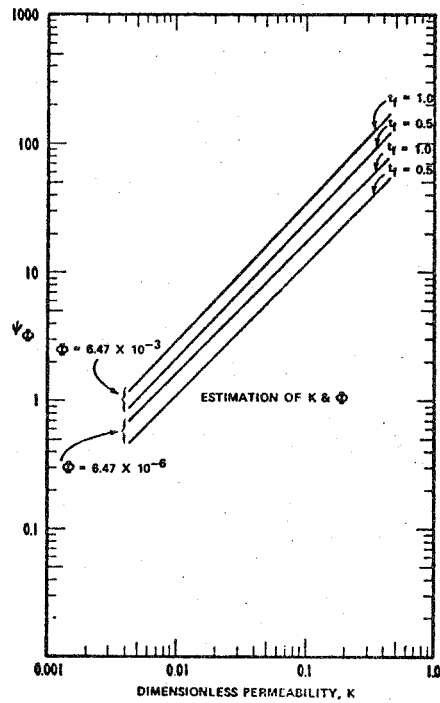


Fig. 4 - ψ_ϕ as a function of dimensionless permeability. Homogeneous reservoir. Estimation of both K and ϕ .

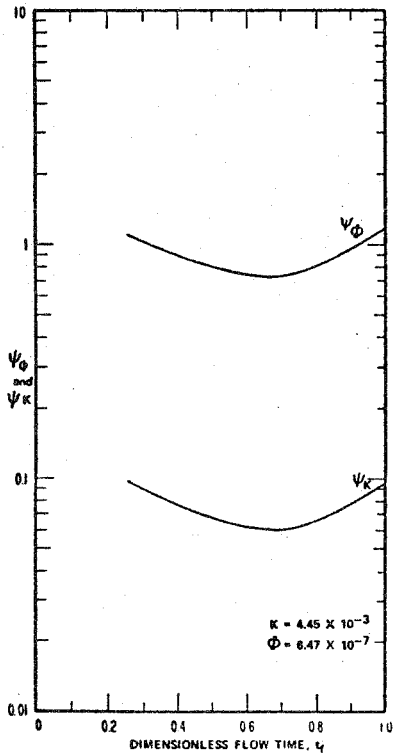


Fig. 5 - ψ_K and ψ_ϕ as functions of dimensionless flow time. Homogeneous reservoir. Estimation of both K and ϕ .

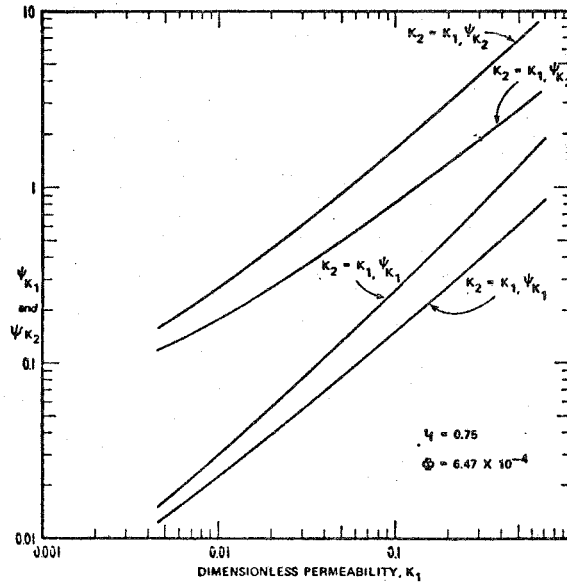


Fig. 6 - ψ_{K_1} and ψ_{K_2} as functions of K_1 . Logarithmically changing dimensionless permeability. Estimation of both K_1 and K_2 .

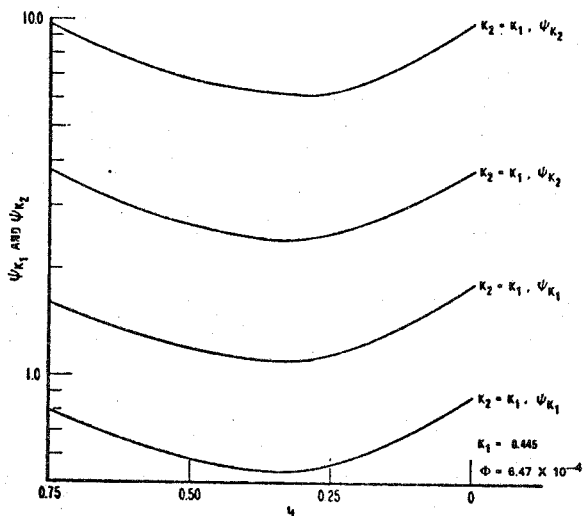


Fig. 7 - ψ_{K_1} and ψ_{K_2} as functions of t_2 . Estimation of both K_1 and K_2 .

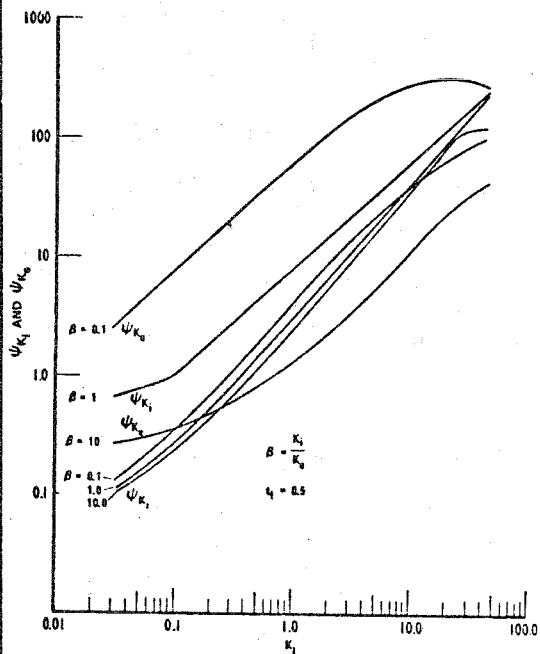


Fig. 8 - ψ_{K_1} and ψ_{K_2} as functions of K_1 . Estimation of both K_1 and K_2 .

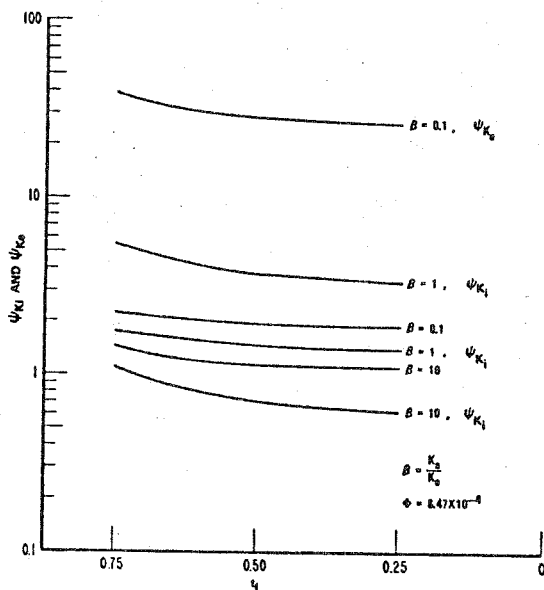


Fig. 9 - ψ_{K_1} and ψ_{K_2} as functions of t_2 . Estimation of both K_1 and K_2 .

Chapter III
ESTIMATION OF SPATIALLY-VARYING PARAMETERS IN
PARTIAL DIFFERENTIAL EQUATIONS

1. Introduction

All of the results in Chapter II deal with the estimation of constant parameters in partial differential equations. Many important physical systems have parameters which vary over the domain of the system. Perhaps one of the most important examples of this type of system is a petroleum reservoir, in which the permeability, porosity, and thickness generally vary throughout the reservoir. To date most of the reported approaches to estimate spatially varying parameters are to divide the space of interest into zones, in each of which the parameter is considered to be constant, thereby converting the problem into the estimation of constant parameters. From the previous chapter we can see that if there are a large number of zones the computing effort required may be prohibitive for practical application. Ideally, we would like to be able to estimate the parameters as a continuous function of spatial position as, in fact, they are.

In this chapter optimal control theory in conjunction with the method of steepest descent is proposed to estimate spatially varying parameters in partial differential equations. In this approach the parameters to be estimated are considered as control variables which are by nature continuous functions of position. This method may considerably reduce the computing time over the existing methods. The

extension of this approach to estimate time-varying or time and spatially varying parameters is straightforward.

In the body of this chapter we present only the general formulation of the problem. The detailed derivation and application to estimate the permeability distribution in a two-dimensional, one-phase petroleum reservoir are given in Appendix III-A and Appendix III-B, respectively. Appendix III-C presents the method for a two-phase petroleum reservoir.

2. General Formulation of the Problem

Let us consider the class of systems described by the partial differential equation

$$u_t(t,x,y) = f(t,x,y,u,u_x,u_y,u_{xx},u_{yy},k(x,y),k_x(x,y),k_y(x,y)) \quad (1)$$

where $u(t,x,y)$ is the n -dimensional state vector; u_x , u_{xx} , and k_x are partial derivatives with respect to x ; u_y , u_{yy} , and k_y are partial derivatives with respect to y ; and k is a p -dimensional vector of spatially varying parameters. The initial state of the system is given by

$$u(0,x,y) = u_0(x,y) \quad x,y \in \Omega \quad (2)$$

where Ω denote the fixed spatial domain of the system, and the boundary conditions are given by

$$g(t,u,u_x,u_y,k) = 0 \quad x,y \in \partial\Omega \quad (3)$$

The observations of the system consist of the m -dimensional vector $Y(x,y,t)$, related to the state by

$$Y(x,y,t) = h(x,y,t,u(x,y,t)) + (\text{errors}) \quad \begin{array}{l} 0 \leq t \leq T \\ x,y \in \Omega + \partial\Omega \end{array} \quad (4)$$

where the observations $Y(x,y,t)$ may be continuous functions of x , y , and t or carried out only at a discrete number of spatial points and a discrete number of times.

The estimation problem is to determine the parameter $k(x,y)$ such that some measure of the difference between the predicted and observed data is a minimum. A popular objective function which will be employed here is the least-square functional

$$J = \int_0^T \iiint_{\Omega} \iiint_{\Omega} [Y(x,y,t) - h(x,y,t,u)]^T Q(x,y,r,s,t) [Y(r,s,t) - h(r,s,t,u)] dr ds dx dy dt \quad (5)$$

where $Q(x,y,r,s,t)$ is an $m \times m$ positive definite weighting matrix, and $Y(x,y,t)$ is a continuous function of x , y , and t . If $Y(x,y,t)$ is a discrete function of x , y , and t , the integrations in (5) are replaced by summations. In (5) $u(x,y,t)$ denotes the solution of (1)-(3) for a given $k(x,y)$.

A close examination of this formulation of the estimation problem reveals that the problem of parameter estimation is intimately related to certain optimal control problems. In fact this problem can be considered formally as an optimal control problem: It is desired to

determine the control policy $k(x,y)$ over the domain Ω such that J is minimized subject to the constraints (1)-(3). Therefore, the optimal control approach can be used to solve the estimation problem. The detailed derivations are given in Appendices III-A and III-B.

Appendix III-A

INT. J. CONTROL, 1972, VOL. 15, NO. 3, 487-495

Estimation of spatially varying parameters in partial differential equations†

W. H. CHEN and J. H. SEINFELD

Department of Chemical Engineering,
California Institute of Technology, Pasadena, California 91109

[Received 21 April 1971]

The estimation of a vector of unknown spatially varying parameters in non-linear partial differential equations from noisy observations is considered. Two algorithms are presented. The first is a method of steepest descent based on consideration of the unknown parameter vector as a control vector. The second is based on treating the parameter as an additional state vector and employing least-square filtering. Computational results are presented on the estimation of the diffusivity in the heat equation.

1. Introduction

The estimation of constant parameters in partial differential equations from noisy observations has recently received attention (Beck 1970 a, b, Fairman and Shen 1970, Phillipson 1971, Seinfeld and Chen 1971). We consider here the estimation of spatially varying parameters in partial differential equations, as arising, for example, in the estimation of the thermal diffusivity of an anisotropic medium or in the estimation of the permeability of a reservoir from pressure measurements at wells. Some special linear cases of this problem have been considered by Cannon (1963, 1968). We consider the general problem of estimating a vector of unknown spatially varying parameters in non linear partial differential equations (P.D.E.'s) from noisy observations of the system state.

We assume the system is governed by the general P.D.E.:

$$x_t = f(t, r, x, x_r, x_{rr}, k, k_r), \quad (1)$$

where $x(r, t)$ is the n -dimensional state vector, t is the time variable, r is the spatial variable, defined on the normalized domain $[0, 1]$, x_t denotes $\partial x / \partial t$, etc. The p -dimensional parameter vector k is assumed to be a function of r only. The initial condition for eqn. (1) is assumed known:

$$x(r, 0) = x_0(r) \quad (2)$$

and the boundary conditions are expressed in the general form:

$$g_0(t, x, x_r) = 0, \quad r = 0, \quad (3)$$

$$g_1(t, x, x_r) = 0, \quad r = 1. \quad (4)$$

The observations of the system are given by the m -dimensional vector $y(r, t)$. The observations are related to the state by:

$$y(r, t) = h(r, t, x(r, t)) + (\text{errors}), \quad (5)$$

where the observations $y(r, t)$ may be continuous functions of r and t or carried out only at a discrete number of spatial locations, r_1, \dots, r_S , and a discrete number of times, t_1, \dots, t_R .

† Communicated by Dr. A. T. Fuller.

The problem is to determine $k(r)$ such that some measure of the difference between the predicted and observed data is a minimum. A popular objective function is the least-square functional:

$$J = \int_0^T \int_0^1 \int_0^1 [y(r, t) - h(r, t, x)]^T Q(r, s, t) [y(s, t) - h(s, t, x)] ds dr dt, \quad (6)$$

where $Q(r, s, t)$ is an $m \times m$ positive semi-definite weighting matrix. This form is for the case in which $y(r, t)$ is a continuous function of r and t . If $y(r, t)$ is a discrete function of r and t , the integrations in eqn. (6) are replaced by summations. In eqn. (6), $x(r, t)$ represents the solution of eqns. (1)–(4) for a given $k(r)$.

There are essentially two ways to approach this problem. The first is to approximate $k(r)$ by a function of r of known form containing a number of unknown constant coefficients. Then the problem becomes one of estimating a set of constant parameters in partial differential equations. In order to simulate $k(r)$ accurately a large number of coefficients may be required. Since this approach is well-developed, we will not consider it further.

The second approach deals directly with $k(r)$ as a function of r . $k(r)$ may be considered either a control variable or an additional state variable. In either case the objective is to choose k to minimize J subject to eqns. (1)–(5). If k is treated as a control variable, the problem becomes one of the optimal control of a distributed parameter system with a control variable that is time independent. On the other hand, if k is considered an additional state variable, state estimation or filtering, techniques applicable to partial differential equations can be used. The only differences between the two ways of treating k lie in the final algorithms for estimating k . We will now develop these two approaches.

2. Method of steepest descent

The method of steepest descent is a popular one for the solution of the two-point boundary value problems arising in the optimal control of lumped and distributed parameter systems (Denn 1969). In this section we derive a method of steepest descent to determine $k(r)$ to minimize J subject to eqns. (1)–(5). Let us begin by defining the additional state variable $x_{n+1}(t)$ by:

$$x_{n+1,t} = \int_0^1 \int_0^1 [y(r, t) - h(r, t, x)]^T Q(r, s, t) [y(s, t) - h(s, t, x)] ds dr, \quad (7)$$

$$x_{n+1}(0) = 0. \quad (8)$$

Thus, $x_{n+1}(T) = J$. Henceforth, the state vector x and the function f will have dimension $n + 1$, with f_{n+1} equal to the right-hand side of eqn. (7).

Let us find the perturbation in $x_{n+1}(T)$ resulting from a perturbation δk in k in order to develop a method of steepest descent. Corresponding to a perturbation δk is a perturbation δx , governed by:

$$\delta x_t = f_x \delta x + f_{x_r} \delta x_r + f_{x_{rr}} \delta x_{rr} + f_k \delta k + f_{k_r} \delta k_r, \quad (9)$$

$$g_{(0)x} \delta x + g_{(0)x_r} \delta x_r = 0, \quad r = 0, \quad (10)$$

$$g_{(1)x} \delta x + g_{(1)x_r} \delta x_r = 0, \quad r = 1. \quad (11)$$

Introduce the $(n + 1)$ -dimensional adjoint vector $\psi(r, t)$ and form the inner product of ψ and eqn. (9) to obtain:

$$(\psi^T \delta x)_t = \psi_t^T \delta x + \psi^T f_x \delta x + \psi^T f_{x_r} \delta x_r + \psi^T f_{x_{rr}} \delta x_{rr} + \psi^T f_k \delta k + \psi^T f_{k_r} \delta k_r. \quad (12)$$

Integrating both sides of eqn. (12) over r from 0 to 1 we obtain:

$$\begin{aligned} \left[\int_0^1 \psi^T \delta x dr \right]_t &= \int_0^1 [\psi_t^T + \psi^T f_x - (\psi^T f_{x_r})_r + (\psi^T f_{x_{rr}})_{rr}] \delta x dr \\ &+ \int_0^1 [\psi^T f_k - (\psi^T f_{k_r})_r] \delta k dr \\ &+ [\psi^T f_{x_r} - (\psi^T f_{x_{rr}})_r] \delta x \Big|_{r=0}^{r=1} \\ &+ \psi^T f_{x_{rr}} \delta x_r \Big|_{r=0}^{r=1} + \psi^T f_{k_r} \delta k \Big|_{r=0}^{r=1}. \end{aligned} \quad (13)$$

Let us define the adjoint vector $\psi(r, t)$ by the following equations:

$$\psi_t^T = -\psi^T f_x + (\psi^T f_{x_r})_r - (\psi^T f_{x_{rr}})_{rr}, \quad (14)$$

$$\psi_i(r, T) = 0, \quad i = 1, 2, \dots, n, \quad (15)$$

$$\psi_{n+1}(T) = 1, \quad (16)$$

$$\psi^T f_{x_r} - (\psi^T f_{x_{rr}})_r - \psi^T f_{x_{rr}} g_{(0)x_r}^{-1} g_{(0)x} = 0, \quad r = 0, \quad (17)$$

$$\psi^T f_{x_r} - (\psi^T f_{x_{rr}})_r - \psi^T f_{x_{rr}} g_{(1)x_r}^{-1} g_{(1)x} = 0, \quad r = 1, \quad (18)$$

Using eqns. (14)–(18) in eqn. (13) we obtain:

$$\left[\int_0^1 \psi^T \delta x dr \right]_t = \int_0^1 [\psi^T f_k - (\psi^T f_{k_r})_r] \delta k dr + \psi^T f_{k_r} \delta k \Big|_{r=0}^{r=1}. \quad (19)$$

Integrating eqn. (19) from 0 to T ;

$$\int_0^1 \psi^T \delta x dr \Big|_{t=T} = \int_0^T \int_0^1 [\psi^T f_k - (\psi^T f_{k_r})_r] \delta k dr dt + \int_0^T \psi^T f_{k_r} \delta k \Big|_{r=0}^{r=1} dt. \quad (20)$$

However, from eqns. (15) and (16), the left-hand side of eqn. (20) is simply $\delta x_{n+1}(T)$, or, equivalently, δJ . The order of integration can be interchanged in eqn. (20) to yield:

$$\delta J = \int_0^1 \left\{ \int_0^T [\psi^T f_k - (\psi^T f_{k_r})_r + \psi^T f_{k_r} \delta(r-1) - \psi^T f_{k_r} \delta(r)] dt \right\} \delta k dr, \quad (21)$$

where $\delta(r)$ is the Dirac delta function.

This is our desired result, namely the perturbation in J resulting from a perturbation in k . Since we want to minimize J , we want to choose δk such that δJ is non-positive. Therefore, we choose:

$$\delta k(r) = -W(r) \left\{ \int_0^T [\psi^T f_k - (\psi^T f_{k_r})_r + \psi^T f_{k_r} \delta(r-1) - \psi^T f_{k_r} \delta(r)] dt \right\}^T, \quad (22)$$

where $W(r)$ is a positive-definite $p \times p$ weighting matrix. Because of the definition of x_{n+1} , only the first n components of ψ and f will enter into the computation of eqn. (22).

Summarizing, the method of steepest descent is as follows:

1. Make an initial guess $k^{(0)}(r)$ and choose a weighting matrix $W(r)$.
2. Solve eqns. (1)–(4) from $t = 0$ to $t = T$. Evaluate J . Then solve eqns. (14)–(18) from $t = T$ to $t = 0$.
3. Compute δk from eqn. (22).
4. Repeat step 2. Continue until subsequent changes in J are less than a preset criterion, $(J^{(i)} - J^{(i+1)})/J^{(i)} \leq \epsilon$.

3. Filtering in distributed systems

Filtering in linear distributed systems with white noise disturbances has been considered by Balakrishnan and Lions (1967), Tzafestas and Nightingale (1968, 1969 a), Meditch (1969), Thau (1969) and Kushner (1970), wherein results analogous to the Kalman filter were obtained. Filtering in non-linear distributed systems has been considered by Tzafestas and Nightingale (1969 b), Seinfeld *et al.* (1969, 1970 a, b), Hwang *et al.* (1971) and Lamont and Kumar (1971). A general non-linear filter, applicable to both boundary and volume disturbances, has been derived by Hwang *et al.* (1971) based on an optimal control approach and invariant embedding.

If we adjoin to eqn. (1) the p relations:

$$k_i = 0 \tag{23}$$

and define the $(n + p)$ -dimensional state vector z as $(x^T, p^T)^T$, then eqn. (1) takes the form:

$$z_t = F(r, t, z, z_r, z_{rr}), \tag{24}$$

where $F = (f^T, 0)^T$. The initial condition for eqn. (24) is:

$$z_i(r, 0) = x_{0i}(r), \quad i = 1, 2, \dots, n, \tag{25}$$

$$z_i(r, 0) = ?, \quad i = n + 1, \dots, n + p. \tag{26}$$

The boundary conditions, eqns. (3) and (4), then apply to the first n components of z .

The optimal least-squares filtering problem is to determine $z(T)$ such that J is minimized, subject to eqns. (3), (4) and (24)–(26). If we denote the optimal filtering estimate by $\hat{z}(r, t)$, then the filter is (Hwang *et al.* 1971):

$$\begin{aligned} \hat{z}_t &= F(r, t, \hat{z}, \hat{z}_r, \hat{z}_{rr}) \\ &+ \int_0^1 \int_0^1 P(r, \zeta, T) h_z^T(\zeta, T, \hat{z}) Q(\zeta, \nu, T) [y(\nu, T) - h(\nu, T, \hat{z})] d\zeta d\nu, \end{aligned} \tag{27}$$

$$\begin{aligned} P_t(r, \rho, t) &= \hat{F}_z^T(r) P + P \hat{F}_z^T(\rho) + \hat{F}_{z_r}(r) P_r + P_\rho F_{z_\rho}^T(\rho) + \hat{F}_{z_{rr}} P_{rr} + P_{\rho\rho} \hat{F}_{z_{\rho\rho}}^T \\ &+ \int_0^1 \int_0^1 P(r, \zeta, T) V(\zeta, \nu, T) P(\nu, s, T) d\zeta d\nu, \end{aligned} \tag{28}$$

$$V(\zeta, \nu, T) = [h_z^T(\zeta, T, \hat{z}) Q(\zeta, \nu, T) (y(\nu, T) - h(\nu, T, \hat{z}))]_z, \tag{29}$$

$$\hat{z}(r, 0) = \hat{z}_0(r), \tag{30}$$

$$g_0(t, \hat{z}, \hat{z}_r) = 0, \quad r = 0, \tag{31}$$

$$g_1(t, \hat{z}, \hat{z}_r) = 0, \quad r = 1, \tag{32}$$

$$P(r, \rho, 0) = P_0(r, \rho), \tag{33}$$

$$g_{(0)z} P(r, \rho, t) + g_{(0)z_r} P_r(r, \rho, t) = 0, \quad r = 0, \tag{34}$$

$$g_{(1)z} P(r, \rho, t) + g_{(1)z_r} P_r(r, \rho, t) = 0, \quad r = 1, \tag{35}$$

where the initial conditions, $\hat{z}_0(r)$ and $P_0(r, \rho)$, must be guessed *a priori*, and $P(r, \rho, t) = P(\rho, r, t)^T$.

The problem of estimating $k(r)$ has now been converted into the problem of estimating $z(r, t)$ given the noisy data, $y(r, t)$, $0 \leq t \leq T$. Of course, since the initial conditions for the first n components of z are known, eqn. (25), the filter will, in effect, be estimating only $k(r)$, the last p elements of z . As we note, the filter requires the solution of $n + p$ state estimate equations, eqn. (27) and $(n + p)^2$ auxiliary Riccati-type equations, eqn. (28). Even though the filter of eqns. (27)–(35) will, in principle, yield estimates for $k(r)$, if the dimension of either x or k is large the computing required to solve eqns. (27) and (28) may be prohibitive.

4. Estimation of the diffusivity in the heat equation

Let us consider the problem of estimating $k(r)$ in the heat equation:

$$x_t = (kx_r)_r, \tag{36}$$

$$x(r, 0) = x_0(r), \tag{37}$$

$$x(0, t) = 0, \tag{38}$$

$$x(1, t) = 1, \tag{39}$$

from discrete noisy measurements of $x(r, t)$ at S locations:

$$y(r_i, t) = x(r_i, t) + (\text{errors}), \quad i = 1, 2, \dots, S. \tag{40}$$

In order to test the two algorithms we will assume that the true value of k is:

$$k(r) = 1 + r \tag{41}$$

and generate the noisy observations by:

$$y(r_i, t) = x(r_i, t) * [1 + aG(0, \sigma)], \quad i = 1, 2, \dots, S, \tag{42}$$

where $x(r_i, t) *$ is the solution of eqns. (36)–(39) and (41) and $G(0, \sigma)$ is a normally distributed random variable with mean zero and standard deviation σ .

Using this example we will study several questions related to the two algorithms developed for estimating k :

- (1) The effect of the number of measurement locations S .
- (2) The effect of the level of the observation noise, a and σ .
- (3) The effect of the choice of the weighting matrices $Q(r, s, t)$ and $W(r)$.

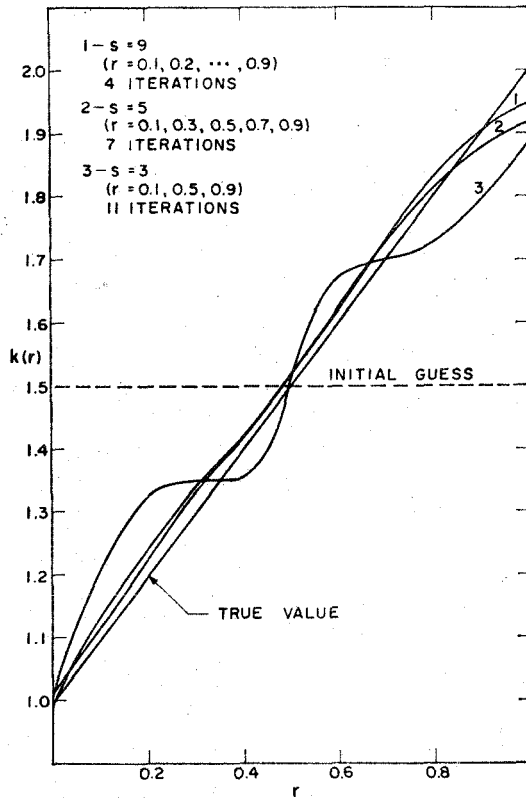
Let us consider first the results using the method of steepest descent. We take the initial condition $x_0(r) = r^2$ and $T = 0.2$. For simplicity, we take $Q(r, s, t)$ to be a function of r and s only, since we will assume that there is no reason to weigh measurements at different times differently. In particular, we will use the form $Q = \exp(-q|r - s|)$, since the strongest weighting in J should naturally occur when $r = s$. The selection of $W(r)$ deserves some consideration. In this example, eqn. (22) reduces to:

$$\delta k = W(r) \int_0^T \psi_r x_r dt. \tag{43}$$

The initial condition $x_0(r)$ may serve as a guide-line for the form of $W(r)$. We presume that we want δk from eqn. (43) to be the same order of magnitude at

all r . Since we know $x_0(r)$, we can compute dx_0/dr as a rough guide to x_r . For $x_0(r) = r^2$, x_r increases with r . Therefore, we would want $W(r)$ to decrease with r . The absolute magnitude of $W(r)$ can only be determined by trial. Both constant values and decreasing functions of r were used for $W(r)$ in the present study. It was found that the accuracy of the estimates is not too sensitive to the choice of $W(r)$.

Fig. 1



Effect of the number of spatial measurements S on the estimated value of $k(r)$ using the method of steepest descent.

Figure 1 shows the effect of the number of measurement locations, S , on the estimated value of $k(r)$. The following parameters were used in generating these results: $q = 15$, $\epsilon = 0.01$, $a = 0$, $\sigma = 0$ and

$$W(r) = \begin{cases} 80 - 120r, & 0 \leq r \leq 0.25, \\ 50, & 0.25 \leq r \leq 1, \end{cases} \quad (44)$$

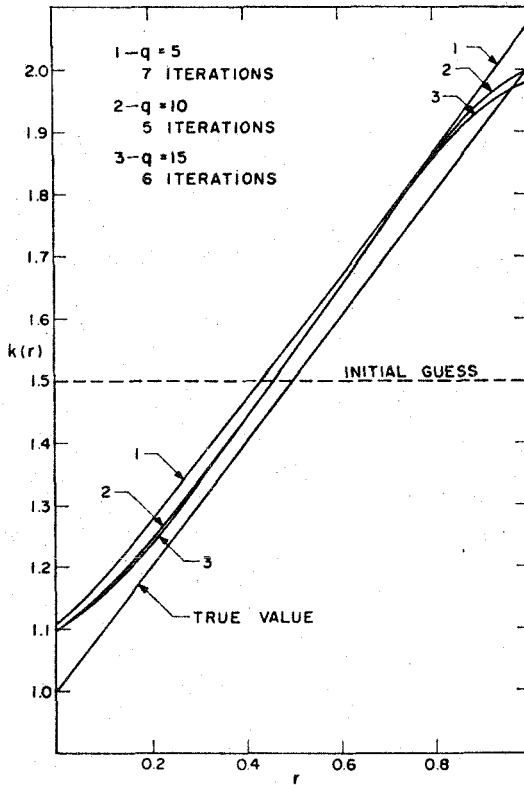
Indicated on fig. 1 are the locations of the measurements and the number of iterations for the three cases. We note, as we would expect, that the accuracy of the estimates decreases as S decreases.

Next, the effect of the level of measurement noise was studied with $q = 15$, $\epsilon = 0.01$, $S = 9$ and $W(r)$ given by eqn. (44). The three cases, $a = 0$, $\sigma = 0$; $a = 0.1$, $\sigma = 0.1$; and $a = 0.3$, $\sigma = 0.3$, were studied. It was found that there

was essentially no effect on the estimated $k(r)$ of the level of noise at these levels (0, 3 and 9%), for which reason we have not shown the results, which closely conform with curve one in fig. 1.

Finally, the effect of Q was considered. Figure 2 shows the $k(r)$ profiles for $q = 5, 10$ and 15 , with $S = 9, \epsilon = 0.01, a = 0, \sigma = 0$ and $W = 50$. Although as q increases, the accuracy of the estimate increases, it does not appear to be a significant effect. From results not shown it was also found that as S decreases, Q must be increased. The choice of Q becomes more important as S decreases.

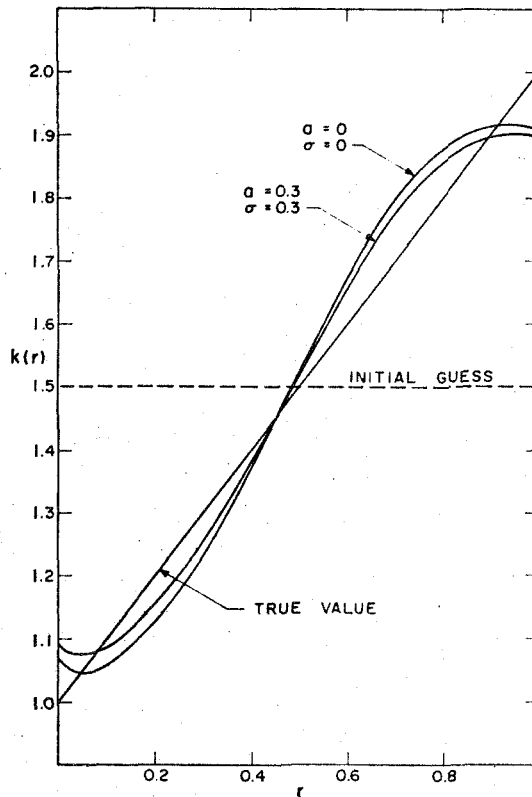
Fig. 2



Effect of the value of q in $Q(r, s, t) = \exp(-q|r-s|)$ on the estimated value of $k(r)$ using the method of steepest descent.

Figure 3 presents the results of estimating $k(r)$ by the non-linear filter. In this case $x_0(r)$ was taken as $\sin \pi r$, and five measurement locations ($S = 5$) were used: $r = 0.1, 0.3, 0.5, 0.7$ and 0.9 . Two curves are shown in fig. 3. The one labelled $a = 0, \sigma = 0$ corresponds to error-free observations, while the curve labelled $a = 0.3, \sigma = 0.3$ corresponds to a 9% error. As we see, there is not a significant difference between the two cases, as we have already observed in the method of steepest descent. Because the non-linear filter requires a solution of the matrix Riccati partial differential equation in two spatial variables, it is not as efficient for parameter estimation as the steepest descent algorithm, which only requires solution of the n -dimensional adjoint equation. Nevertheless, the results shown in fig. 3 indicate that the non-linear filter can be used to estimate parameters in P.D.E.

Fig. 3



Effect of the level of error on $\hat{k}(T)$ at $T = 0.2$ using the non-linear filter.

5. Summary

Two algorithms for the estimation of spatially varying parameters in non-linear P.D.E. have been presented. The method of steepest descent appears to be computationally more efficient than non-linear filtering because fewer P.D.E. must be integrated in steepest descent. Both algorithms were applied to estimate the diffusivity in the heat equation from discrete noisy state measurements.

ACKNOWLEDGMENT

This work was partially supported by a grant from the Chevron Oil Field Research Company.

REFERENCES

- BALAKRISHNAN, A. V., and LIONS, J. L., 1967, *J. Compt. Syst. Sci.*, **1**, 391.
 BECK, J. V., 1970 a, *J. bas. Engng*, **92**, 215.
 BECK, J. V., 1970 b, *Int. J. Heat Mass Transfer*, **13**, 703.
 CANNON, J. R., 1968, *SIAM J. Numer. Anal.*, **5**, 257.
 CANNON, J. R., and JONES, B. F., JR., 1963, *Int. J. Engng Sci.*, **1**, 457.
 DENN, M. M., 1969, *Optimization by Variational Methods* (New York: McGraw-Hill).
 FAIRMAN, F. W., and SHEN, D. N. C., 1970, *Int. J. Control*, **11**, 929.
 HWANG, M., SEINFELD, J. H., and GAVALAS, G. R., 1971, *J. math. Analysis Applic.* (in press).

- KUSHNER, A. J., 1970, *J. SIAM Control*, **8**, 346.
- LAMONT, G. B., and KUMAR, K. S. P., 1971, *J. math. Analysis Applic.* (in press).
- MEDITCH, J. S., 1969, Boeing Scientific Research Laboratory Report D1-82-0917.
- PHILLIPSON, G. A., 1971, *Identification of Distributed Systems* (New York: American Elsevier).
- SEINFELD, J. H., 1969, *Chem. Engng Sci.*, **24**, 75.
- SEINFELD, J. H., and CHEN, W. H., 1971, *Chem. Engng. Sci.* **26**, 753.
- SEINFELD, J. H., GAVALAS, G. R., and HWANG, M., 1970 a, Joint Automatic Control Conference (Georgia Institute of Technology, Atlanta, Georgia).
- SEINFELD, J. H., and HWANG, M., 1970 b, *Chem. Engng Sci.*, **25**, 741.
- THAU, F. E., 1969, *J. bas. Engng, Trans. A.S.M.E.*, Series D91, **1**, 73.
- TZAFESTAS, S. G., and NIGHTINGALE, J. M., 1968, *Proc. Instn elect. Engrs*, **115**, 1207.
- TZAFESTAS, S. G., and NIGHTINGALE, J. M., 1969 a, *Electronics Letts*, **5**, 199.
- TZAFESTAS, S. G., and NIGHTINGALE, J. M., 1969 b, *Proc. Instn elect. Engrs*, **116**, 1085.

Appendix III-B

SOCIETY OF PETROLEUM ENGINEERS OF AIME
6200 North Central Expressway
Dallas, Texas 75206

PAPER NUMBER SPE 4545

THIS IS A PREPRINT --- SUBJECT TO CORRECTION

A New Algorithm for Automatic History Matching

By

Wen H. Chen, George R. Gavalas and John H. Seinfeld, California Institute of Technology

© Copyright 1973
American Institute of Mining, Metallurgical, and Petroleum Engineers, Inc.

This paper was prepared for the 48th Annual Fall Meeting of the Society of Petroleum Engineers of AIME, to be held in Las Vegas, Nev., Sept. 30-Oct. 3, 1973. Permission to copy is restricted to an abstract of not more than 300 words. Illustrations may not be copied. The abstract should contain conspicuous acknowledgment of where and by whom the paper is presented. Publication elsewhere after publication in the JOURNAL OF PETROLEUM TECHNOLOGY or the SOCIETY OF PETROLEUM ENGINEERS JOURNAL is usually granted upon request to the Editor of the appropriate journal provided agreement to give proper credit is made.

Discussion of this paper is invited. Three copies of any discussion should be sent to the Society of Petroleum Engineers office. Such discussion may be presented at the above meeting and, with the paper, may be considered for publication in one of the two SPE magazines.

ABSTRACT

A new algorithm is presented for the determination of reservoir parameters, such as permeability and porosity, from well pressure measurements. The key feature of the algorithm is that reservoir properties are considered as continuous functions of position rather than as uniform in a certain number of zones. The method, based on an optimal control formulation of the history matching problem, may offer significant savings in computing time over conventional gradient optimization methods, such as steepest descent and Gauss-Newton. A numerical example is presented to illustrate the use of the method and its comparison to other algorithms.

INTRODUCTION

The process of determining unknown parameter values, such as permeability and porosity, in a mathematical reservoir model, that give the closest fit of measured and calculated pressures is commonly called "history matching." Knowing the reservoir properties, one can then use the mathematical model (or, simulator) to explore various future production policies that optimize some economic criterion of performance. The simplest approach to history-matching is a trial and error procedure of visually examining the output of each simulator run and adjusting one or more of the parameters by intuition or References and illustrations at end of paper.

experience and trying again. Large portions of the time and cost of a simulator study are often attributable to history matching, particularly when a trial and error procedure is used. In principle, one would like an automatic routine, applicable to simulators of varying complexity, one that will not require inordinate amounts of computing time to achieve a set of parameter estimates.

In recent years a number of authors have investigated the subject of history matching¹⁻⁸. All of the reported approaches involve dividing the reservoir into a number of zones, in each of which the properties to be estimated are assumed to be uniform. (These zones may, in fact, correspond to the spatial grid employed for the finite-difference solution of the simulator.) Then the history matching problem becomes that of determining the parameter values in each of, say, N zones, k_1, k_2, \dots, k_N , such that some measure (usually a sum of squares) of the deviation between calculated and observed pressures is minimized. A typical measure of deviation is

$$J = \int_0^T \sum_{j=1}^M [p^{obs}(r_j, t) - p^{cal}(r_j, t)]^2 dt \dots (1)$$

where $p^{obs}(r_j, t)$ and $p^{cal}(r_j, t)$ are the observed and calculated pressures at the j th well, which

is at location $r_j = (x_j, y_j)$, $j = 1, 2, \dots, M$, and T is the total time period over which observations are available. For the case of measurements made at discrete times the performance index can be defined as follows. If we have n_1 measurements at well 1 at n_1 different times, n_2 measurements at well 2 at n_2 different times, ..., and n_M measurements at well M at n_M different times, we define the performance index as

$$J = \sum_{j=1}^M \sum_{i=1}^{n_j} [p^{obs}(r_j, t_{ij}) - p^{cal}(r_j, t_{ij})]^2 \dots (2)$$

This index can be placed in the form of Eq. (1) as follows

$$J = \int_0^T \sum_{j=1}^M \sum_{i=1}^{n_j} [p^{obs}(r_j, t) - p^{cal}(r_j, t)]^2 \delta(t - t_{ij}) dt \dots (3)$$

where $\delta(\cdot)$ is the Dirac delta function.

Since Eq. (2) can be written in the form of Eq. (1), we shall henceforth take Eq. (1) as the general performance index for history matching.

To perform the minimization of Eq. (1), most methods rely on some type of gradient optimization procedure. Two common methods of iteratively improving an initial guess of the N unknown parameters are the steepest descent method and the Gauss-Newton method. In the former method, the $(j+1)$ st iterate of k_i , k_i^{j+1} , is determined from

$$k_i^{j+1} = k_i^j + \gamma \frac{\partial J}{\partial k_i} \dots (4)$$

where $\gamma < 0$ and $\partial J / \partial k_i$ can be determined from Eq. (1) by

$$\frac{\partial J}{\partial k_i} = -2 \int_0^T \sum_{j=1}^M [p^{obs}(r_j, t) - p^{cal}(r_j, t)] \frac{\partial p^{cal}(r_j, t)}{\partial k_i} dt \dots (5)$$

In the Gauss-Newton method, on the other hand, we assume that each k_i differs from the initial guess by an amount Δk_i and that the calculated pressure can be expanded in a Taylor series about the initial guess,

$$p^{cal}(r_j, t; k_1 + \Delta k_1, \dots, k_N + \Delta k_N) = p^{cal}(r_j, t; k_1, \dots, k_N)$$

$$+ \sum_{l=1}^N \frac{\partial p^{cal}(r_j, t; k_1, \dots, k_N)}{\partial k_l} \Delta k_l \dots (6)$$

We can substitute Eq. (6) into Eq. (1), making J a function of the Δk_i . Then setting $\partial J / \partial \Delta k_i = 0$ yields N simultaneous linear equations for the Δk_i , the solution of which yields the recursion formula

$$k_i^{j+1} = k_i^j + \gamma (R^{-1})_i \left(\frac{\partial J}{\partial k} \right)^T \dots (7)$$

where $(R^{-1})_i$ is the i th row of the $N \times N$ matrix R^{-1} , where the i, l element of R is defined by

$$R_{il} = \left(2 \int_0^T \sum_{j=1}^M \frac{\partial p^{cal}(r_j, t)}{\partial k_i} \frac{\partial p^{cal}(r_j, t)}{\partial k_l} dt \right) \dots (8)$$

and $\frac{\partial J}{\partial k} = \left[\frac{\partial J}{\partial k_1}, \frac{\partial J}{\partial k_2}, \dots, \frac{\partial J}{\partial k_N} \right]$, an N -dimensional row vector.

We note that R represents an approximation to H , where H is the Hessian matrix. This can be seen from the definition of Hessian matrix:

$$H_{il} = \frac{\partial^2 J}{\partial k_i \partial k_l} = \left(2 \int_0^T \sum_{j=1}^M \frac{\partial p^{cal}(r_j, t)}{\partial k_i} \frac{\partial p^{cal}(r_j, t)}{\partial k_l} dt - 2 \int_0^T \sum_{j=1}^M [p^{obs}(r_j, t) - p^{cal}(r_j, t)] \frac{\partial^2 p^{cal}(r_j, t)}{\partial k_i \partial k_l} dt \right) \dots (9)$$

If the second term is neglected, in the hope that the residue is small, then R is a good approximation to H . When $R = H$, we have the so-called Newton method⁹. The high cost of computing second order derivatives leads one to make use of simplifications of the Newton method, such as the Gauss-Newton method. Reported computational results indicate that the Gauss-Newton method is one of the most efficient gradient methods¹⁰.

We note that in both of these methods above it is necessary to compute the sensitivity coefficients, $\partial p^{cal} / \partial k_i$, $i = 1, 2, \dots, N$, i.e. the first partial derivative of pressure with respect to each parameter. The sensitivity coefficients can be computed, in principle, in several ways:

1. Make a simulator base run with all N parameters at their initial values. Then,

perturbing each parameter a small amount, make an additional simulator run for each parameter in the system. Sensitivity coefficients may then be determined using the finite difference formula,

$$\frac{\partial p^{cal}(r, t)}{\partial k_i} = \frac{\{ p^{cal}(r, t; k_1, k_2, \dots, k_{i-1}, k_i + \Delta k_i, k_{i+1}, \dots, k_N) - p^{cal}(r, t; k_1, \dots, k_N) \}}{\Delta k_i} \dots \dots \dots (10)$$

2. Derive a set of "sensitivity equations" from the original partial differential equations describing the reservoir system. In this new set of equations in partial differential form, the dependent variables will be the sensitivity coefficients. The finite difference equivalent of the sensitivity equations will then be solved simultaneously with the original pressure equation. A closely related alternative would be to derive sensitivity equations from the finite difference form of the simulator equations.

3. Assume that the difference between the observed and calculated pressures is a linear function of the parameters⁴. That is

$$p^{obs}(r_j, t_j) - p^{cal}(r_j, t_j) = a_{j0} + \sum_{i=1}^N a_{ji} k_i$$

$j = 1, \dots, I \dots \dots \dots (11)$

where I is the total number of measurements. Therefore, the sensitivity coefficients become independent of the parameter values. Experience with real problems, however, has indicated that the sensitivity coefficients are not constant over a wide range of parameter values, and, consequently, this approach is not a generally valid one for history-matching.

With N parameters, method 1 requires N + 1 simulator runs for each step in the iteration of improving the guesses. Method 2 also requires the solution of N + 1 partial differential equations per iteration (1 simulator run plus N sensitivity equations). Herein lies the basic computational inefficiency in the multi-zonal approach to history-matching when N is large, namely the large number of repetitive solutions of partial differential equations that are required in each iteration.

In this paper we propose a new approach to the history-matching problem which is designed

to circumvent the excessive computational requirements of standard methods. In essence, we treat the reservoir property being estimated, say permeability, as a *continuous* function of location rather than as one assuming discrete values in a number of zones. To solve the problem we seek that *function*, for example, $k(x,y)$, that minimizes the objective function J. Such an approach is, of course, in keeping with the probable physical nature of an actual reservoir. The key feature of the new approach is that it requires the solution of only two partial differential equations per iteration (one simulator run plus one adjoint equation) no matter how fine the spatial resolution.

The method we present is essentially a gradient optimization method, in which an initial guess $k^0(x,y)$ is improved iteratively. However, the treatment of the unknown property as a function as opposed to a set of constant parameters enables us to avoid the sensitivity equations arising in the multi-zone approach.

In the next section the method is summarized. Then follows a computational example illustrating the use of the method and giving a detailed comparison of this new algorithm to two conventional constant zone approaches, steepest descent and the Gauss-Newton method, for a single-phase hypothetical reservoir. The full derivation of the algorithm for a single-phase reservoir is presented in Appendix A. Although the method is presented only for the single-phase case, it is applicable in principle to two-phase simulators. To conserve space, we have not presented the derivation for this latter case here.

SUMMARY OF THE ALGORITHM FOR A SINGLE-PHASE RESERVOIR

Let us consider a reservoir of uniform thickness h but arbitrary cross section and containing L producing (or injecting) wells and M-L observing wells (with zero production rates). The radius and production flow rate of the jth well will be denoted by r_{wj} and q_j , respectively. The simulator equation for the pressure in a reservoir containing a single-phase fluid can be written (we drop the superscript *cal* for convenience)

$$\frac{\partial p}{\partial t} = \nabla \cdot (\alpha(r) \nabla p) \quad r \in S \dots \dots \dots (12)$$

where $\alpha(r) = k(r)/\phi\mu c$ is the hydraulic diffusivity, (ϕ is assumed constant), ∇ is the two-dimensional gradient operator with respect to the position vector r , and S denotes the region of the plane occupied by the reservoir. $k(r)$ denotes the unknown property, presumed to be the permeability, which is a function of position r . Boundary conditions are given on the

boundaries B_{w_j} of each well and on the external boundary B_e of the reservoir as follows

$$\frac{\partial p}{\partial z} = 0 \quad \underline{r} \in B_{w_j}, \quad j = 1, 2, \dots, L \quad \dots (13)$$

$$h \int_{B_{w_j}} \frac{k(\underline{r})}{\mu} \frac{\partial p}{\partial n} d\ell = q_j \quad \underline{r} \in B_{w_j}, \quad j = 1, 2, \dots, L \quad (14)$$

$$\frac{\partial p}{\partial z} = 0 \quad \underline{r} \in B_{w_j}, \quad j = L + 1, \dots, M \quad (15)$$

$$h \int_{B_{w_j}} \frac{k(\underline{r})}{\mu} \frac{\partial p}{\partial n} d\ell = 0 \quad \underline{r} \in B_{w_j}, \quad j = L + 1, \dots, M \quad \dots (16)$$

$$\frac{\partial p}{\partial n} = 0 \quad \underline{r} \in B_e \quad \dots (17)$$

where $\partial p/\partial n$ and $\partial p/\partial z$ are the normal and tangential derivatives to the indicated boundary, either B_{w_j} or B_e . Eqs. (13) and (15) specify that the pressure on the periphery of the j th well is uniform, while Eqs. (14) and (16) specify the production rate in terms of an integral of the flux. Eq. (17) states that the outer boundary of the reservoir is impermeable. The initial condition to Eq. (12) can be taken as some specified distribution,

$$p(\underline{r}, 0) = p_o(\underline{r}) \quad \dots (18)$$

We have assumed that the reservoir contains M wells at coordinate location $\underline{r}_1, \dots, \underline{r}_M$. The observed pressures at each of the M wells will be denoted by $p^{obs}(\underline{r}_j, t)$. The history matching problem is to determine $k(\underline{r})$ to minimize an objective function related to the discrepancy between model and data. A common form of such a function and the one which we shall employ, is given by Eq. (1).

Concisely stated, we wish to minimize J , given by Eq. (1), subject to Eqs. (12)-(18). We wish to develop a gradient optimization method which will iteratively improve an initial guess $k^0(\underline{r})$ by

$$k^{j+1}(\underline{r}) = k^j(\underline{r}) + \delta k^j(\underline{r}) \quad \dots (19)$$

This can be done by a variational approach, such as commonly used in optimal control theory¹¹. The full derivation of the method

is given in the Appendix. The final result is that $\delta k^j(\underline{r})$ is computed by

$$\delta k^j(\underline{r}) = W(\underline{r}) \phi \mu c \int_0^T [(\nabla \psi) \cdot (\nabla p)] dt \quad \dots (20)$$

where $W(\underline{r})$ is a positive weighting function and $\psi(\underline{r}, t)$ is governed by the boundary value problem (note that a final condition at $t = T$ appears rather than an initial condition at $t = 0$):

$$\frac{\partial \psi}{\partial t} = -\nabla \cdot (\alpha(\underline{r}) \nabla \psi) \quad \underline{r} \in S \quad \dots (21)$$

$$\psi(\underline{r}, T) = 0 \quad \dots (22)$$

$$\frac{\partial \psi}{\partial z} = 0 \quad \underline{r} \in B_{w_j}, \quad j = 1, \dots, M \quad \dots (23)$$

$$h \int_{B_{w_j}} \frac{k(\underline{r})}{\mu} \frac{\partial \psi}{\partial n} d\ell = 2h\phi c [p^{obs}(\underline{r}, t) - p(\underline{r}, t)] \quad \underline{r} \in B_{w_j}, \quad j = 1, \dots, M \quad \dots (24)$$

$$\frac{\partial \psi}{\partial n} = 0 \quad \underline{r} \in B_e \quad \dots (25)$$

The algorithm is used as follows:

1. Make an initial guess $k^0(\underline{r})$ and solve Eqs. (12)-(18). Evaluate J by Eq. (1).
2. Compute $\psi(\underline{r}, t)$ by solving Eqs. (21)-(25) from $t = T$ to $t = 0$.
3. Compute $\delta k(\underline{r})$ by Eq. (20) and update $k^j(\underline{r})$ by $k^{j+1}(\underline{r}) = k^j(\underline{r}) + \delta k^j(\underline{r}) \quad j = 0, 1, 2, \dots$
4. If a convergence criterion

$$\frac{J^j - J^{j+1}}{J^j} \leq \epsilon$$

is met, stop; if not, return step 1 with k^{j+1} in place of k^0 .

We now present a detailed application of the algorithm to the estimation of the permeability distribution in a hypothetical single-phase reservoir. In addition, we compare the performance of the algorithm to that of conventional steepest descent and Gauss-Newton methods.

APPLICATION OF THE METHOD

We consider the estimation of the permeability distribution $k(x,y)$ in the single-phase reservoir shown in Fig. 1, the pressure in which is governed by

$$\frac{\partial p}{\partial t} = \frac{1}{c\phi\mu} \left\{ \frac{\partial}{\partial x} \left(k(x,y) \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left(k(x,y) \frac{\partial p}{\partial y} \right) \right\} \quad (26)$$

$$p(x,y,0) = p_0 \quad 0 \leq x \leq L_1, \quad 0 \leq y \leq L_2 \quad \dots \quad (27)$$

$$\frac{\partial p}{\partial x} = 0 \quad x = 0, L_1 \quad \dots \quad (28)$$

$$\frac{\partial p}{\partial y} = 0 \quad y = 0, L_2 \quad \dots \quad (29)$$

$$h \int_B \frac{k}{\mu} \frac{\partial p}{\partial n} d\ell = q \quad (\text{injection well}) \quad \dots \quad (30)$$

$$h \int_{B_j} \frac{k}{\mu} \frac{\partial p}{\partial n} d\ell = 0 \quad (\text{observing wells}) \quad \dots \quad (31)$$

$j = 1, 2, \dots, 8$

The locations of the injection and observation wells are shown in Fig. 1. The true but presumed unknown permeability was chosen as

$$k(x,y) = 0.02 + \frac{0.7}{L_1} \sqrt{x^2 + y^2} \quad \dots \quad (32)$$

Observed pressures were generated by solving Eqs. (26)-(31) numerically with Eq. (32) and the following parameter values: $\phi = 0.2$, $h = 1$ ft., $L_1 = 60,000$ ft., $L_2 = 30,000$ ft., $c = 1.72 \times 10^{-5}$ psi⁻¹, $\mu = 0.352$ cp., $p_0 = 0$ and $q = 500$ ft³ day⁻¹ (injection). The alternating direction implicit method was used to solve the state (p) and adjoint (ψ) equations.

The problem is to estimate $k(x,y)$ from the observed pressures. The objective function used is

$$J = \sum_{i=1}^K \sum_{j=1}^M [p^{\text{obs}}(x_j, y_j, t_i) - p(x_j, y_j, t_i)]^2 \quad (33)$$

where K discrete time measurements ($K = 20$) are assumed to be available at each of the eight ($M = 8$) observation wells. Note that no pressure data are taken at the injection well.

Three techniques will be used to solve this problem:

1. Steepest descent method of Eqs. (4) and (5);
2. Gauss-Newton method of Eqs. (7),(8), and (5); and
3. The new algorithm developed in this paper (the variational method).

For the first two methods it is necessary to divide the reservoir into zones in each of which the permeability is taken to be constant. We shall consider two cases, 4 zones and 8 zones, assuming that k is constant in each zone. Thus, we have 4 unknown parameters in the 4 zone case and 8 unknown parameters in the 8 zone case. The configuration of the 8 zones is shown in Fig. 1, while Fig. 2 shows the location of the 4 zones. Sensitivity coefficients for the steepest descent and Gauss-Newton methods were computed numerically by Eq. (10) by changing each of the k_i one at a time by 5% of its value and then calculating the corresponding change in p .

Some typical results are summarized in Table 1. Of particular interest in the comparison among the three methods are two points:

1. The performance of the method, i.e. how rapidly J was decreased; and
2. The computing time requirements of the method, i.e. how many seconds of computing time were required per iteration and for comparable reductions in the objective function J .

We see that each of the three methods reduced J by a factor of about 100 in 10 or fewer iterations. However, from the standpoint of computing time, the variational method was superior to each of the other two methods in the cases of both 4 and 8 zones. Since the final value of J is different for each method, for the purpose of comparison we can choose a value of J , say 13, at which to compare the methods. Since the number of iterations needed to reach a given value of J is different for different initial guesses, the time reported will be the average time for $k^0 = 0.2$ and $k^0 = 0.7$. Under these conditions the variational method takes 55 seconds (5 iterations for $k^0 = 0.2$ and 3 iterations for $k^0 = 0.7$), the Gauss-Newton method takes 77 seconds (3 iterations for $k^0 = 0.2$ and 5 iterations for $k^0 = 0.7$) for the 4-zone case and 100 seconds (2 iterations for $k^0 = 0.2$ and 5 iterations for $k^0 = 0.7$) for the 8-zone case, and the steepest descent method takes 137 seconds (10 iterations for $k^0 = 0.2$

and 5 iterations for $k^0 = 0.7$) for the 4-zone case and 144 seconds (5 iterations for both $k^0 = 0.2$ and $k^0 = 0.7$) for the 8-zone case.

Figs. 3 and 4 compare for the observation wells 2 and 8 the observed and calculated pressures for the initial guess, the tenth iteration for the variational method, and the tenth iteration for the method of steepest descent for the 4-zone case. The final pressures for the 8-zone case by the methods of steepest descent and Gauss-Newton are approximately the same as the final pressures calculated by the variational method. The final pressures for 4-zone case by the methods of steepest descent and Gauss-Newton are approximately the same. As we expected, the 8-zone case is superior to the 4-zone case in terms of pressure-matching. This can be seen from Figs. 3 and 4.

Fig. 5 presents the distribution of permeability at $y = 9000$ ft. and 21,000 ft. for the initial guess, the tenth iteration for the variational method, the tenth iteration for the 8-zone and 4-zone cases by the method of steepest descent, and the average value of the true permeability in each zone. The average value in each zone is defined by

$$k_i = \frac{\int \int k(x,y) dx dy}{\int \int dx dy} \quad i = 1, \dots, 8$$

We can draw some interesting conclusions from the results in Table 1 and Figs. 3-5. We note that in each case the least-square criterion J has been reduced significantly in a few iterations; likewise, the pressure histories after a few iterations are very close to the observed pressures. Nevertheless, there is little correspondence between the final values of k in the 8 zones in the two constant-zone cases, as can be seen in Table 1. Therefore, in spite of the fact that the three methods perform well in decreasing J , the parameter values determined by the separate methods bear no real relation to each other. The key problem is that the pressure histories at the observation wells are relatively insensitive to variations in $k(x,y)$. This becomes particularly apparent when the reservoir is divided arbitrarily into zones, zones which may bear no relation to the true $k(x,y)$ form in the reservoir, and the final k values in these zones differ depending on the experiment. More precisely, the reservoir system is relatively unobservable with respect to $k(x,y)$.

The results obtained in the present study thus serve to point out a problem of perhaps greater intrinsic importance than history matching algorithm development, namely the problem

of the initial choice of the number and type of parameters to be estimated in a history matching exercise. Thus, it is important that the selection of reservoir properties to be determined be commensurate with the quantity and quality of the data available. This problem has not been treated here--it remains as one for future efforts¹³.

CONCLUSIONS

A new history matching method designed to overcome the excessive computational requirements of standard methods is presented. The key feature of the method is that the reservoir property being estimated is treated as a continuous function of location rather than as one assuming discrete values in a number of zones. In a hypothetical exercise the new method performed comparably to two standard constant-zone gradient methods with respect to reduction of the least-square performance index, but doing so with a smaller expenditure of computing time. In the example, both four and eight uniform zones were employed. In actual practice, more than 100 zones are often used for large reservoirs. While the computing time for standard constant-zone methods increases directly with the number of zones (or parameters), because of the required sensitivity coefficients, that for the variational method presented here does not change since constant zones are not employed. Thus, while the computing time for the variational method was about one-half of that for the 8-zone gradient methods, for, say, 64 zones, the computational savings of the new method over a conventional method should be a factor of 16.

ACKNOWLEDGMENT

This work was supported by a grant from the Chevron Oil Field Research Company.

REFERENCES

1. Jacquard, P. and Jain, C.: "Permeability Distributions from Field Pressure Data," Soc. Pet. Eng. Jour. (December 1965) vol. 5, 281-294.
2. Jahns, H. O.: "A Rapid Method for Obtaining a Two-Dimensional Reservoir Description from Well Pressure Response Data," Soc. Pet. Eng. Jour. (December 1966) vol. 6, 315-327.
3. Brill, J. P., Burgoyne, A. T. and Dixon, T. N.: "Numerical Simulation of Drillstem Tests as an Interpretation Technique," Jour. Pet. Tech. (November 1969) 1413-1420.

4. Coats, K. H., Dempsey, J. R., and Henderson, J. H.: "A New Technique for Determining Reservoir Description from Field Performance Data," Soc. Pet. Eng. Jour. (March 1970) vol. 10, 66-74.
5. Slater, G. E. and Durrer, E. J.: "Adjustment of Reservoir Simulation Models to Match Field Performance," Soc. Pet. Eng. Jour. (September 1971) vol. 11, 295-305.
6. Thomas, L. K., Hellums, L. J., and Reheis, G. M.: "A Nonlinear Automatic History Matching Technique for Reservoir Simulation Models," Soc. Pet. Eng. Jour. (December 1972) vol. 12, 508-514.
7. Veatch, R. W., Jr. and Thomas, G. W.: "A Direct Approach for History Matching," Soc. Pet. Eng. Preprint No. 3515 (October 1971).
8. Carter, R. D., Kemp, L. F., Jr., Pierce, A. C. and Williams, D. L.: "Performance Matching with Constraints," Soc. Pet. Eng. Preprint No. 4260 (January 1973).
9. Crockett, J. B. and Chernoff, H.: "Gradient Methods of Maximization," Pacific Jour. Math. (1955) vol. 5, 33.
10. Bard, Y.: "Comparison of Gradient Methods for the Solution of Nonlinear Parameter Estimation Problems," SIAM Jour. Numer. Anal. (1970) vol. 7, 157.
11. Denn, M.M.: "Optimization by Variational Methods," McGraw-Hill, New York (1969).
12. Coats, K. H. and Terhune, M. H.: "Comparison of Alternating Direction Explicit and Implicit Procedures in Two-Dimensional Flow Calculations," Soc. Pet. Eng. Jour. (December 1966) vol. 6, 350.
13. Dixon, T. N., Seinfeld, J. H., Startzman, R.A. and Chen, W. H.: "Reliability of Reservoir Parameters from History Matched Drillstem Tests," paper SPE 4282 presented at SPE Third Numerical Simulation of Reservoir Performance Symposium, Houston, Texas, Jan. 10-13, 1973.

APPENDIX A

DERIVATION OF THE METHOD

In this appendix we derive the basic equations of the new method for a single-phase reservoir, that is, a simulator consisting of a single partial differential equation.

Let us consider a reservoir of uniform thickness h but arbitrary cross section and containing L producing wells and $M-L$ observing wells (with zero production rates). The simulator equations for the pressure are given by Eqs. (12)-(18). Although we shall consider here the estimation of $k(r)$, the method is sufficiently general so that other unknown properties, say porosity ϕ , could be treated in an analogous manner. The history-matching problem is to determine $k(r)$ to minimize an

objective function related to the discrepancy between model and data. A common form of such an objective function, and the one which we shall employ, is given by Eq. (1). Since we assume that the pressure on the periphery of each well is constant, we can rewrite Eq. (1) as

$$J = \sum_{j=1}^M \frac{1}{2\pi r_w j} \int_0^T \int_{B_{w_j}} [p^{obs}(r,t) - p(r,t)]^2 d\Omega dt \dots \dots \dots (A-1)$$

Concisely stated, we wish to minimize J , given by Eq. (A-1), subject to Eqs. (12)-(18). This can be done by a variational approach, such as commonly used in optimal control theory¹¹. Using such an approach we shall now derive a steepest descent algorithm which can be used to improve iteratively an initial guess $k^0(r)$ such that J is continually decreased. Basically we desire to relate a perturbation in $k(r)$, $\delta k(r)$, to a perturbation in J , δJ . We then choose a $\delta k(r)$ such that δJ is always negative.

The change in $p(r,t)$, δp , resulting from a change in $k(r)$, and hence $\alpha(r)$, is given by the solution of

$$\frac{\partial \delta p}{\partial t} = \nabla \cdot (\delta \alpha(r) \nabla p) + \nabla \cdot (\alpha(r) \nabla \delta p) \quad (A-2)$$

We introduce a so-called adjoint variable $\psi(r,t)$ and multiply Eq. (A-2) by ψ to give

$$\frac{\partial}{\partial t} (\psi \delta p) = \frac{\partial \psi}{\partial t} \delta p + \psi \nabla \cdot (\delta \alpha(r) \nabla p) + \psi \nabla \cdot (\alpha(r) \nabla \delta p) \dots \dots \dots (A-3)$$

Integrating both sides of Eq. (A-3) over the spatial domain S and over t and using $\delta p(r,0) = 0$, we obtain

$$\int_S \int_0^T \psi \delta p \Big|_T dS = \int_0^T \int_S \frac{\partial \psi}{\partial t} \delta p dS dt + \int_0^T \int_S \psi \nabla \cdot (\delta \alpha(r) \nabla p) dS dt + \int_0^T \int_S \psi \nabla \cdot (\alpha(r) \nabla \delta p) dS dt \dots \dots \dots (A-4)$$

By using the identity,

$$\nabla \cdot (\underline{U}\underline{A}) = (\nabla \underline{U}) \cdot \underline{A} + \underline{U} \nabla \cdot \underline{A} \dots \dots \dots (A-5)$$

Eq. (A-4) becomes

$$\begin{aligned} \iint_S \psi \delta p \Big|_T dS &= \int_0^T \iint_S \left\{ \frac{\partial \psi}{\partial t} \delta p \right. \\ &+ \nabla \cdot (\psi \delta \alpha(\underline{r}) \nabla p) - (\nabla \psi) \cdot (\delta \alpha(\underline{r}) \nabla p) \\ &+ \nabla \cdot (\psi \alpha(\underline{r}) \nabla \delta p) - \nabla \cdot (\delta p \alpha(\underline{r}) \nabla \psi) \\ &\left. + \delta p \nabla \cdot (\alpha(\underline{r}) \nabla \psi) \right\} dS dt \dots \dots \dots (A-6) \end{aligned}$$

Employing the divergence theorem, we obtain

$$\begin{aligned} \iint_S \psi \delta p \Big|_T dS &= \int_0^T \iint_S \frac{\partial \psi}{\partial t} \delta p dS dt \\ &+ \int_0^T \int_{B_e} \psi \delta \alpha(\underline{r}) \frac{\partial p}{\partial n} d\ell dt \\ &- \sum_{j=1}^M \int_0^T \int_{B_{w_j}} \psi \delta \alpha(\underline{r}) \frac{\partial p}{\partial n} d\ell dt \\ &- \int_0^T \iint_S (\nabla \psi \cdot \nabla p) \delta \alpha(\underline{r}) dS dt \\ &+ \int_0^T \int_{B_e} \psi \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} d\ell dt \\ &- \sum_{j=1}^M \int_0^T \int_{B_{w_j}} \psi \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} d\ell dt \\ &+ \int_0^T \iint_S \delta p \nabla \cdot (\alpha(\underline{r}) \nabla \psi) dS dt \\ &- \int_0^T \int_{B_e} \delta p \alpha(\underline{r}) \frac{\partial \psi}{\partial n} d\ell dt \\ &+ \sum_{j=1}^M \int_0^T \int_{B_{w_j}} \delta p \alpha(\underline{r}) \frac{\partial \psi}{\partial n} d\ell dt \dots \dots \dots (A-7) \end{aligned}$$

From Eq. (17) we know that

$$\frac{\partial \delta p}{\partial n} = 0 \quad \underline{r} \in B_e \dots \dots \dots (A-8)$$

Using Eqs. (17) and (A-8), Eq. (A-7) can be written as

$$\begin{aligned} \iint_S \psi \delta p \Big|_T dS &= \int_0^T \iint_S \left\{ \left[\frac{\partial \psi}{\partial t} + \nabla \cdot (\alpha(\underline{r}) \nabla \psi) \right] \delta p \right. \\ &- (\nabla \psi \cdot \nabla p) \delta \alpha(\underline{r}) \left. \right\} dS dt - \int_0^T \int_{B_e} \alpha(\underline{r}) \frac{\partial \psi}{\partial n} \delta p d\ell dt \\ &- \sum_{j=1}^M \int_0^T \int_{B_{w_j}} \psi \left[\alpha(\underline{r}) \frac{\partial \delta p}{\partial n} + \delta \alpha(\underline{r}) \frac{\partial p}{\partial n} \right] d\ell dt \\ &+ \sum_{j=1}^M \int_0^T \int_{B_{w_j}} \alpha(\underline{r}) \frac{\partial \psi}{\partial n} \delta p d\ell dt \dots \dots \dots (A-9) \end{aligned}$$

The change in J, δJ , resulting from a change in $p(\underline{r}, t)$ is given by

$$\begin{aligned} \delta J &= - \sum_{j=1}^M \frac{1}{\pi r_{w_j}} \int_0^T \int_{B_{w_j}} [p^{obs}(\underline{r}, t) \\ &- p(\underline{r}, t)] \delta p d\ell dt \dots \dots \dots (A-10) \end{aligned}$$

Combining Eqs. (A-9) and (A-10) gives

$$\begin{aligned} \iint_S \psi \delta p \Big|_T dS + \delta J &= \int_0^T \iint_S \left\{ \left[\frac{\partial \psi}{\partial t} \right. \right. \\ &+ \nabla \cdot (\alpha(\underline{r}) \nabla \psi) \delta p - (\nabla \psi \cdot \nabla p) \delta \alpha(\underline{r}) \left. \right\} dS dt \\ &- \int_0^T \int_{B_e} \alpha(\underline{r}) \frac{\partial \psi}{\partial n} \delta p d\ell dt \\ &- \sum_{j=1}^M \int_0^T \int_{B_{w_j}} \psi \left[\alpha(\underline{r}) \frac{\partial \delta p}{\partial n} + \delta \alpha(\underline{r}) \frac{\partial p}{\partial n} \right] d\ell dt \\ &+ \sum_{j=1}^M \int_0^T \int_{B_{w_j}} \left\{ \alpha(\underline{r}) \frac{\partial \psi}{\partial n} - \frac{1}{\pi r_{w_j}} [p^{obs}(\underline{r}, t) \right. \end{aligned}$$

$$- p(\underline{r}, t) \} \delta p d\ell dt \dots \dots \dots (A-11)$$

The object of adding δJ to Eq. (A-9) is to obtain a relation between δJ and $\delta\alpha(\underline{r})$. If we can do so, then we can choose $\delta\alpha(\underline{r})$ in such a way as to insure that $\delta J < 0$. In order to determine the relation between δJ and $\delta\alpha(\underline{r})$, let us have $\psi(\underline{r}, t)$ be governed by

$$\frac{\partial \psi}{\partial t} = - \nabla \cdot (\alpha(\underline{r}) \nabla \psi) \dots \dots \dots (A-12)$$

with the final condition

$$\psi(\underline{r}, T) = 0 \dots \dots \dots (A-13)$$

and choose the boundary conditions for Eq. (A-12) such that the second, third, and fourth terms on the right-hand side of Eq. (A-11) vanish. This can be done as follows. Because of the arbitrariness of δp on the boundaries and the uniformity of δp on the inner boundary, B_{w_j} , $j = 1, \dots, M$

$$\int_0^T \int_{B_e} \alpha(\underline{r}) \frac{\partial \psi}{\partial n} \delta p d\ell dt = 0$$

and

$$\sum_{j=1}^M \int_0^T \int_{B_{w_j}} \left\{ \alpha(\underline{r}) \frac{\partial \psi}{\partial n} - \frac{1}{\pi r_{w_j}} [p^{obs}(\underline{r}, t) - p(\underline{r}, t)] \right\} \delta p d\ell dt = 0$$

imply

$$\frac{\partial \psi}{\partial n} = 0 \quad \underline{r} \in B_e \dots \dots \dots (A-14)$$

and

$$\int_{B_{w_j}} \alpha(\underline{r}) \frac{\partial \psi}{\partial n} d\ell = 2[p^{obs}(\underline{r}, t) - p(\underline{r}, t)]$$

$$\underline{r} \in B_{w_j}, j = 1, \dots, M \dots \dots \dots (A-15)$$

respectively. To find the third boundary condition, we need only note that, from Eqs. (14) and (16)

$$\int_{B_{w_j}} \left[\alpha(\underline{r}) \frac{\partial \delta p}{\partial n} + \delta\alpha(\underline{r}) \frac{\partial p}{\partial n} \right] d\ell = 0$$

$$\underline{r} \in B_{w_j}, j = 1, \dots, M \dots \dots \dots (A-16)$$

and that in order for the relation

$$\sum_{j=1}^M \int_0^T \int_{B_{w_j}} \psi \left[\alpha(\underline{r}) \frac{\partial \delta p}{\partial n} + \delta\alpha(\underline{r}) \frac{\partial p}{\partial n} \right] d\ell dt = 0$$

to hold, a sufficient condition is that

$$\frac{\partial \psi}{\partial \ell} = 0 \quad \underline{r} \in B_{w_j}, j = 1, \dots, M \dots \dots (A-17)$$

This is the third boundary condition.

Substituting Eqs. (A-12)-(A-15) and Eq. (A-17) into Eq. (A-11) we obtain

$$\delta J = - \int_0^T \int_S [(\nabla \psi) \cdot (\nabla p)] \delta\alpha(\underline{r}) dS dt \dots \dots (A-18)$$

We can interchange the order of integration as follows:

$$\delta J = - \int_S \int_0^T \left\{ [(\nabla \psi) \cdot (\nabla p)] dt \right\} \delta\alpha(\underline{r}) dS \dots \dots (A-19)$$

In order to decrease J by choice of $\delta\alpha(\underline{r})$ we want $\delta J < 0$. This can be accomplished by setting

$$\delta\alpha(\underline{r}) = W(\underline{r}) \int_0^T [(\nabla \psi) \cdot (\nabla p)] dt \dots \dots \dots (A-20)$$

on, in terms of $k(\underline{r})$,

$$\delta k(\underline{r}) = \phi_{lc} W(\underline{r}) \int_0^T [(\nabla \psi) \cdot (\nabla p)] dt \dots \dots (A-21)$$

where $W(\underline{r})$ is an arbitrary positive function of \underline{r} .

TABLE 1 - COMPARISON OF HISTORY MATCHING RESULTS USING STEEPEST DESCENT
AND GAUSS-NEWTON METHODS AND THE VARIATIONAL METHOD

	Steepest Descent				Gauss Newton				Variational Method	
	8-Zone		4-Zone		8-Zone		4-Zone		k(x,y) = 0.2	k(x,y) = 0.7
Initial quest k_i^0 i=1, ..., 8 for 8-zone i=1, ..., 4 for 4-zone	0.2	0.7	0.2	0.7	0.2	0.7	0.2	0.7		
Initial Value of J*	335.4	187.5	335.4	187.5	335.4	187.5	335.4	187.5	335.4	187.5
Number of Iterations	10	7	10	6	5	10	4	5	10	6
Total Computing Time**(seconds)	284	185	178	96	150	281	76	97	127	76
Computing Time for Each Iteration (seconds)	28.4	26.4	17.8	16.0	30.0	28.1	19.0	19.4	12.7	12.6
Final Value of J	3.2	2.8	13.1	12.6	3.9	3.8	12.5	12.6	6.6	4.4
Vinal Value of k_1	0.124	0.169	0.338	0.346	0.491	0.501	0.339	0.351		
k_2	0.466	0.363	0.430	0.411	0.219	0.225	0.400	0.404		
k_3	0.503	0.410	0.333	0.332	0.291	0.291	0.329	0.346		
k_4	0.504	0.634	0.522	0.553	4.038	4.128	0.585	0.585		
k_5	0.217	0.367			1.942	2.043				
k_6	0.443	0.360			0.241	0.248				
k_7	0.528	0.532			0.374	0.368				
k_8	0.495	0.655			12.367	93.554				

* J is given by Eq. (33)

** IBM 370/155

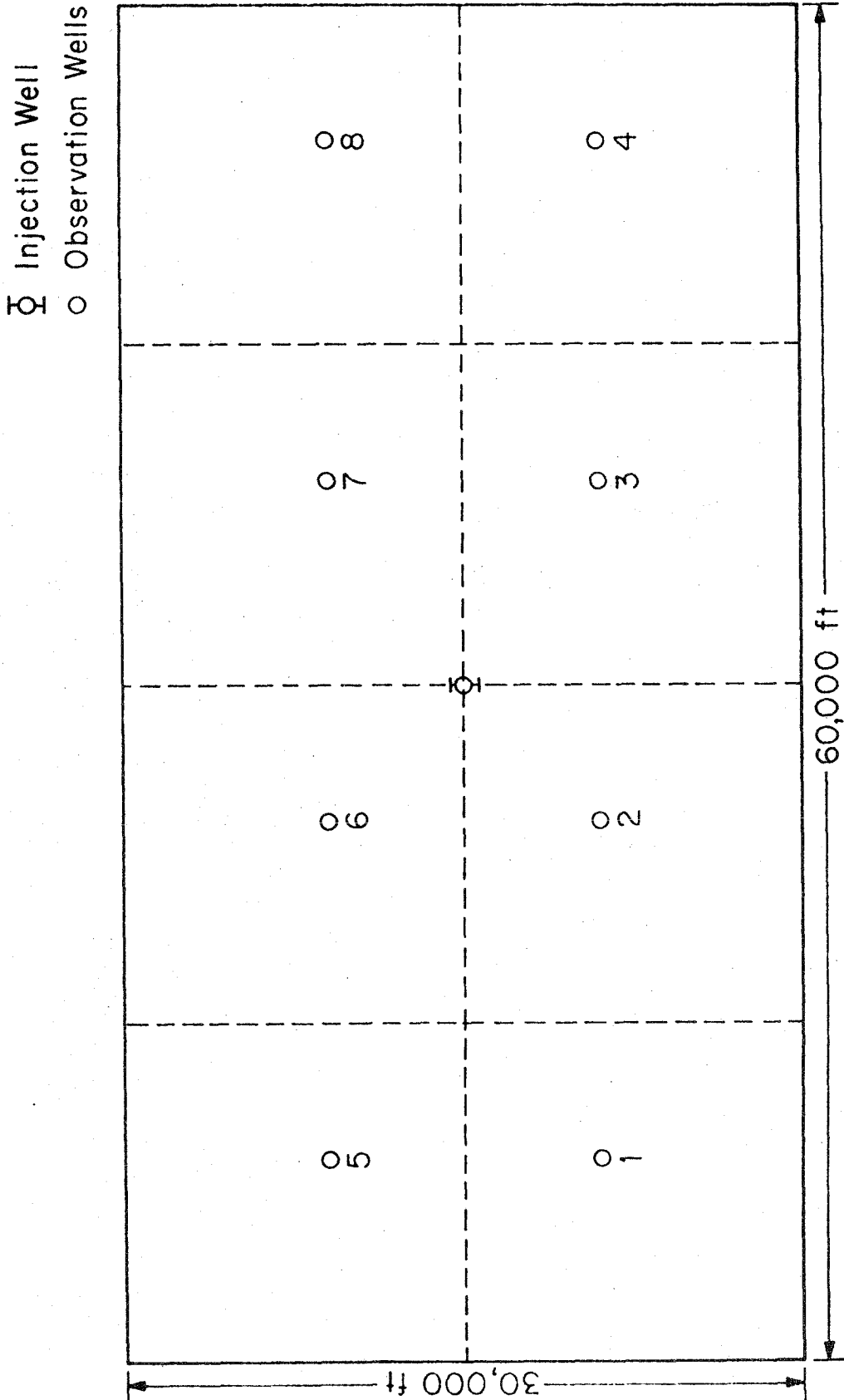


Figure 1: Reservoir with single injection well and eight observing wells (8 zones)

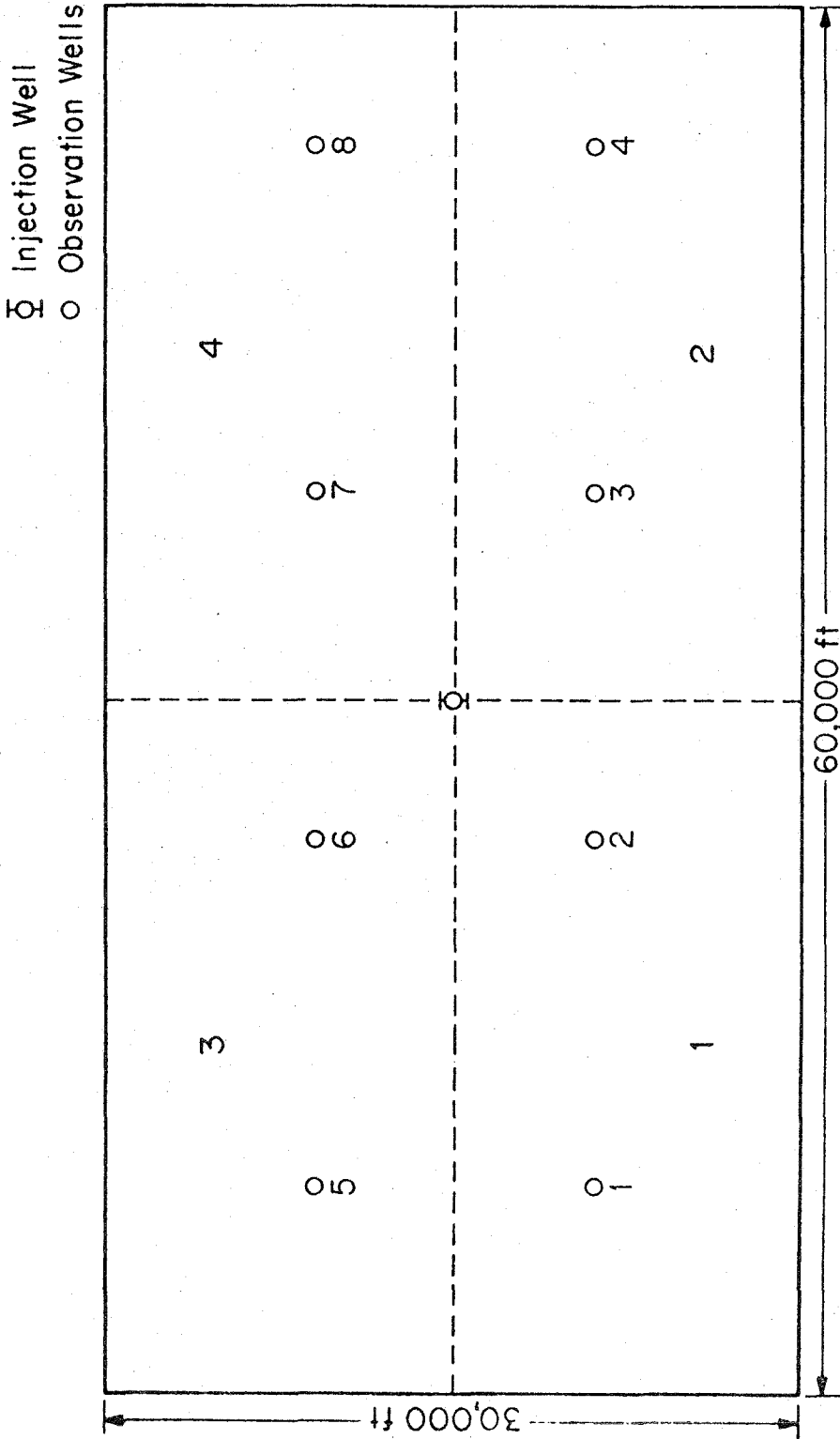


Figure 2: Reservoir with single injection well and eight observing wells (4 zones)

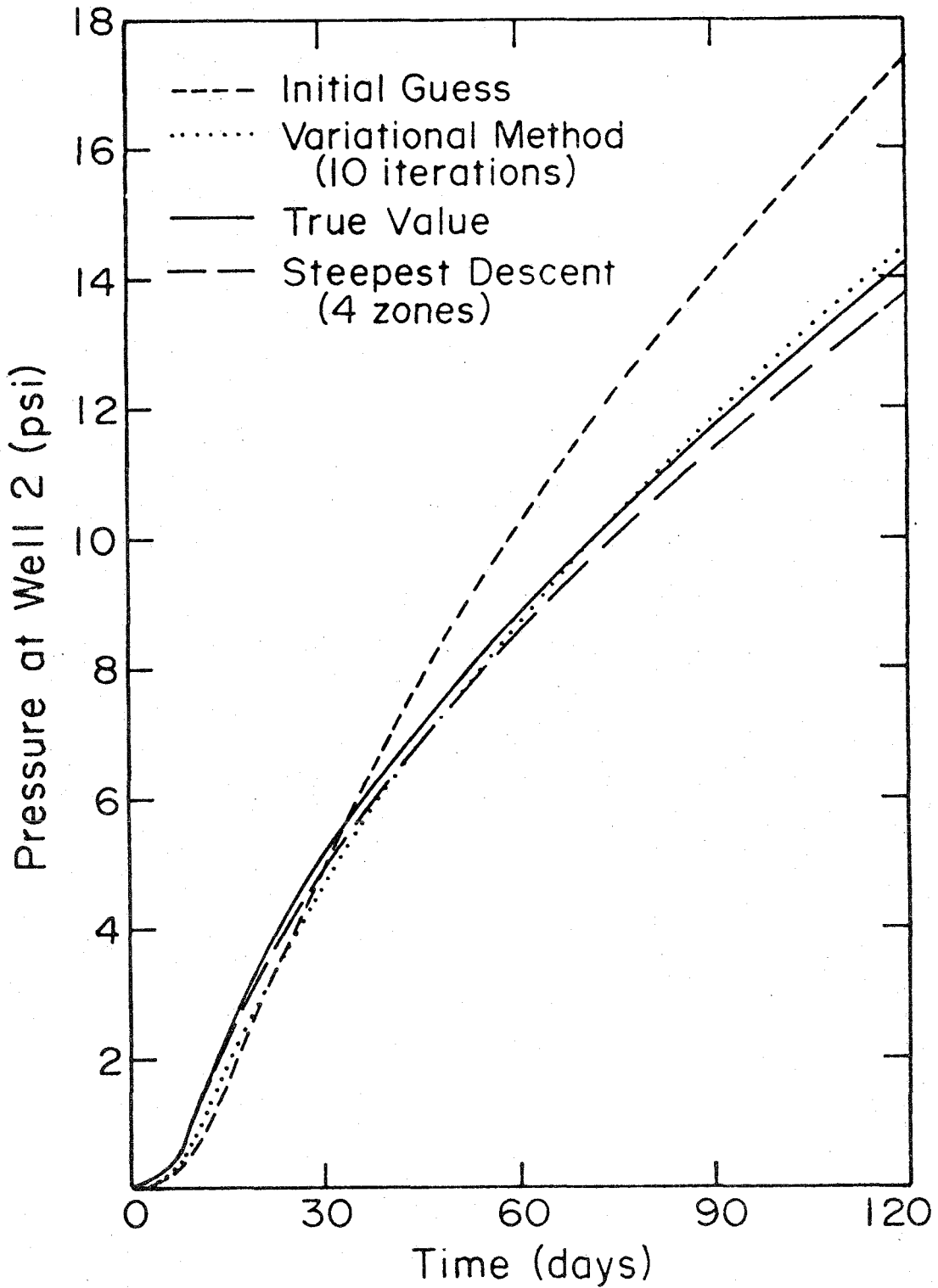


Figure 3: Actual and estimated pressure at Well 2

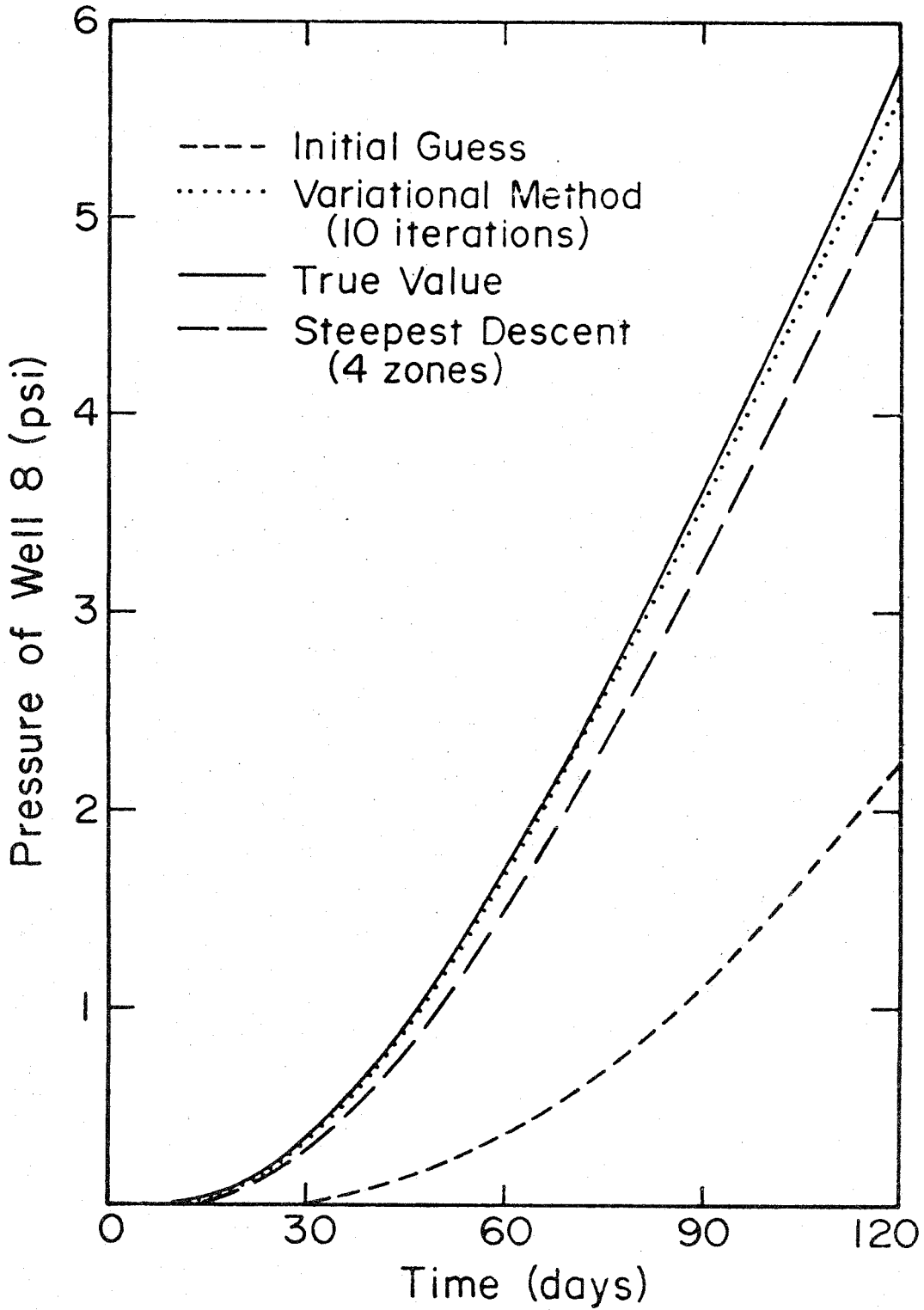


Figure 4: Actual and estimated pressure at Well 8

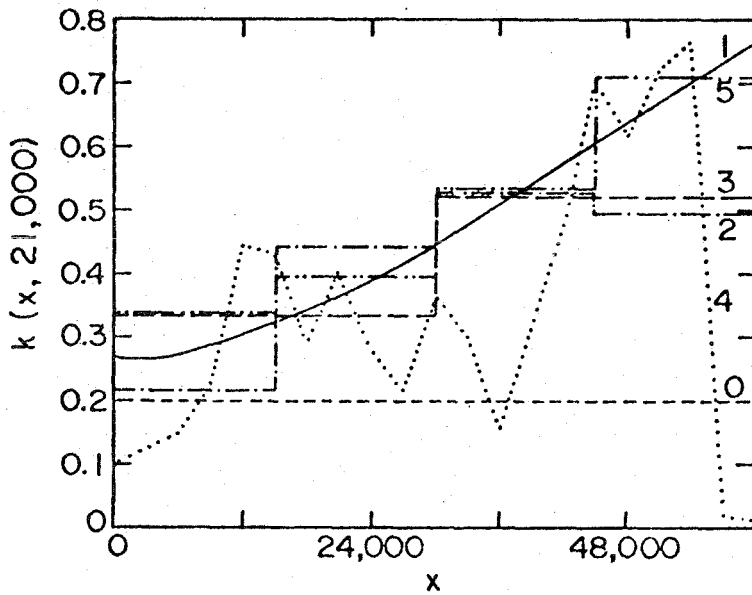
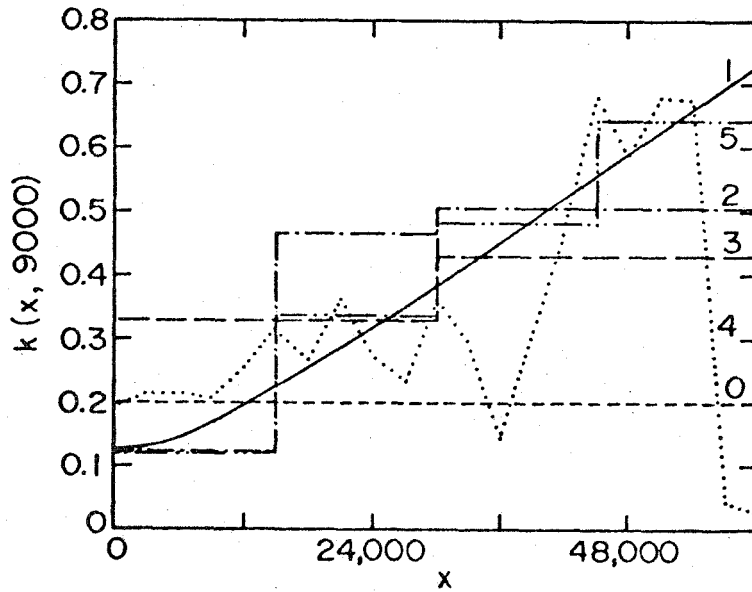


Figure 5: Permeability distributions as a function of x at $y = 9,000$ ft and $21,000$ ft.

- | | |
|--------------------------------|--------------------------------|
| 0 = initial guess | 3 = steepest descent (4 zones) |
| 1 = true value | 4 = variational method |
| 2 = steepest descent (8 zones) | 5 = average value (8 zones) |

Appendix III-C

ESTIMATION OF PARAMETERS IN TWO-PHASE PETROLEUM RESERVOIRS

In this appendix we show that the variational method is applicable to two-phase petroleum reservoirs.

The basic differential equations describing multiphase flow of liquids in petroleum reservoirs have been described in detail by Collins [30] and others. The fundamental development is based on combining the law of mass conservation, Darcy's formula, and the equations of state for each mobile fluid phase. If we ignore capillary pressure differences in the system and also neglect gravity effects, and if x and y are the coordinates of a two-dimensional cartesian system, then the conservation of mass of oil yields in the continuity equation

$$\frac{\partial}{\partial x} \left(\frac{\rho_{os} K_{xo}}{\beta_o \mu_o} \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\rho_{os} K_{yo}}{\beta_o \mu_o} \frac{\partial p}{\partial y} \right) = \frac{\partial}{\partial t} \left(\frac{\phi \rho_{os}}{\beta_o} S_o \right) \quad (\text{III-C.1})$$

and for the conservation of mass of gas

$$\begin{aligned} \frac{\partial}{\partial x} \left[\left(\frac{\rho_g K_{xg}}{\mu_g} + \frac{s \rho_{gs} K_{xo}}{\beta_o \mu_o} \right) \frac{\partial p}{\partial x} \right] + \frac{\partial}{\partial y} \left[\left(\frac{\rho_g K_{yg}}{\mu_g} + \frac{s \rho_{gs} K_{yo}}{\beta_o \mu_o} \right) \frac{\partial p}{\partial y} \right] \\ = \frac{\partial}{\partial t} \left(\phi \rho_g S_g + \frac{\phi s \rho_{gs}}{\beta_o} S_o \right) \end{aligned} \quad (\text{III-C.2})$$

where S_o is oil saturation, S_g is liquid saturation, K_{xo} is effective permeability in the x -direction for oil, K_{yo} is the effective permeability in the y -direction for oil, K_{xg} is effective permeability in the x -direction for gas, K_{yg} is effective permeability in the y -direction for gas, ρ_{os} is the oil density (at atmospheric condition),

μ_o is the viscosity of oil, β_o is the formation volume factor for oil, μ_g is the viscosity of gas, ρ_g is the mass density of gas (at P), ρ_{gs} is the mass density of gas (at atmospheric condition), s is the solubility and ϕ is porosity. These two equations with appropriate initial and boundary conditions in conjunction with $S_o + S_g = 1$ constitute three equations for determining the three quantities P, S_o , and S_g as functions of the space coordinates and time.

Since the absolute permeabilities are the parameters we want to estimate, the effective permeabilities are expressed in terms of absolute permeabilities and relative permeabilities as

$$K_{xo} = K_x k_{ro}$$

$$K_{yo} = K_y k_{ro}$$

$$K_{xg} = K_x k_{rg}$$

and

$$K_{yg} = K_y k_{rg}$$

where K_x and K_y are the absolute permeabilities in the x-direction and the y-direction, and k_{ro} and k_{rg} are the relative permeabilities for oil and gas, respectively. Here we note that the absolute permeabilities K_x and K_y are functions of space coordinates only and the relative permeabilities k_{ro} and k_{rg} are functions of saturation only.

For the sake of simplicity, Eqs. (III-C.1) and (III-C.2) are rewritten as follows:

$$\frac{\partial}{\partial x} [K_x A(p) k_{ro} \frac{\partial p}{\partial x}] + \frac{\partial}{\partial y} [K_y A(p) k_{ro} \frac{\partial p}{\partial y}] = \frac{\partial}{\partial t} [B(p) S_0] \quad (\text{III-C.3})$$

$$\begin{aligned} \frac{\partial}{\partial x} [K_x (C(p) k_{rg} + D(p) k_{ro}) \frac{\partial p}{\partial x}] + \frac{\partial}{\partial y} [K_y (C(p) k_{rg} + D(p) k_{ro}) \frac{\partial p}{\partial y}] \\ = \frac{\partial}{\partial t} [E(p) S_g + F(p) S_0] \end{aligned} \quad (\text{III-C.4})$$

where

$$A(p) = \frac{\rho_{os}}{\beta_o \mu_o}$$

$$B(p) = \frac{\phi \rho_{os}}{\beta_o}$$

$$C(p) = \frac{\rho_g}{\mu_g}$$

$$D(p) = \frac{s \rho_{gs}}{\beta_o \mu_o}$$

$$E(p) = \phi \rho_g$$

$$F(p) = \frac{\phi s \rho_{gs}}{\beta_o}$$

In order that the variational method will be applicable, and for the sake of numerical solution, Eqs. (III-C.3) and (III-C.4) must be modified as follows. Multiplying Eq. (III-C.3) by $E(p) - F(p)$, multiplying Eq. (III-C.4) by $B(p)$, replacing S_0 in Eqs. (III-C.3) and (III-C.4) by $1 - S_g$, and adding up the resulting equations gives

$$\begin{aligned}
 & [E(p) - F(p)] \frac{\partial}{\partial x} [K_x A(p) k_{ro} \frac{\partial p}{\partial x}] + B(p) \frac{\partial}{\partial x} [k_x (C(p) k_{rg} + D(p) k_{ro}) \frac{\partial p}{\partial x}] \\
 & + [E(p) - F(p)] \frac{\partial}{\partial y} [K_y A(p) k_{ro} \frac{\partial p}{\partial y}] + B(p) \frac{\partial}{\partial y} [K_y (C(p) k_{rg} + D(p) k_{ro}) \frac{\partial p}{\partial y}] \\
 & = \{S_g [(E(p) - F(p))' B(p) - (E(p) - F(p)) B'(p)] \\
 & \quad + [E(p) - F(p)] B'(p) + B(p) F'(p)\} \frac{\partial p}{\partial t} \quad \text{(III-C.5)}
 \end{aligned}$$

where $z'(p)$ denote $\frac{dz(p)}{dp}$.

From Eq. (III-C.3) we have

$$\begin{aligned}
 & \frac{\partial}{\partial x} [K_x A(p) k_{ro} \frac{\partial p}{\partial x}] + \frac{\partial}{\partial y} [K_y A(p) k_{ro} \frac{\partial p}{\partial y}] \\
 & = (1 - S_g) B'(p) \frac{\partial p}{\partial t} - B(p) \frac{\partial S_g}{\partial t} \quad \text{(III-C.6)}
 \end{aligned}$$

Let

$$\begin{aligned}
 a(p, S_g) &= S_g [(E(p) - F(p))' B(p) - (E(p) - F(p)) B'(p)] \\
 & \quad + [E(p) - F(p)] B'(p) + B(p) F'(p)
 \end{aligned}$$

$$b(p, S_g) = (1 - S_g) B'(p)$$

$$c(p) = E(p) - F(p)$$

$$d(p, S_g) = A(p) k_{ro} (S_g)$$

$$e(p, S_g) = C(p) k_{rg} (S_g) + D(p) k_{ro} (S_g)$$

then, after some algebraic manipulations, Eqs. (III-C.5) and Eqs. (III-C.6) become

$$\frac{\partial p}{\partial t} = \frac{c}{a} \frac{\partial}{\partial x} (K_x d \frac{\partial p}{\partial x}) + \frac{B}{a} \frac{\partial}{\partial x} (K_x e \frac{\partial p}{\partial x}) + \frac{c}{a} \frac{\partial}{\partial y} (K_y d \frac{\partial p}{\partial y}) + \frac{B}{a} \frac{\partial}{\partial y} (K_y e \frac{\partial p}{\partial y}) \quad (\text{III-C.7})$$

$$\begin{aligned} \frac{\partial S_g}{\partial t} = & \frac{bc}{aB} \frac{\partial}{\partial x} (K_x d \frac{\partial p}{\partial x}) + \frac{b}{a} \frac{\partial}{\partial x} (K_x e \frac{\partial p}{\partial x}) - \frac{1}{B} \frac{\partial}{\partial x} (K_x d \frac{\partial p}{\partial x}) + \frac{bc}{aB} \frac{\partial}{\partial y} (K_y d \frac{\partial p}{\partial y}) \\ & + \frac{b}{a} \frac{\partial}{\partial y} (K_y e \frac{\partial p}{\partial y}) - \frac{1}{B} \frac{\partial}{\partial y} (K_y d \frac{\partial p}{\partial y}) \end{aligned} \quad (\text{III-C.8})$$

Now Eqs. (III-C.7) and (III-C.8) which describe the two-phase, two-dimensional petroleum reservoir flow are in the form of Eq. (1) in Appendix III-A. Thus, the variational method developed in Appendix III-A can be applied to Eqs. (III-C.7) and (III-C.8) for determining the parameters in these two equations.

Chapter IV

ESTIMATION OF THE LOCATION OF THE BOUNDARY OF A DISTRIBUTED REGION WITH APPLICATION TO PETROLEUM RESERVOIRS

1. Introduction

A problem of substantial economic importance to the petroleum production industry is the determination of the size and shape of a reservoir from early pressure data from the initial wells drilled. Seismic data serve to define the probable area occupied by the reservoir; however, a means of using early well pressure data to determine further the volume and shape of the reservoir would be quite valuable.

On the basis of representing the pressure behavior in a single-phase bounded reservoir in terms of an eigenfunction expansion, Gavalas and Seinfeld [40] have shown how the total pore volume of an arbitrary-shaped reservoir can be estimated from late transient pressure data at the available wells. We consider here the related problem of the estimation of the shape (or the location of the boundary) of a reservoir from pressure data at an arbitrary number of wells. This problem is posed in somewhat general terms as optimally estimating the location of the boundary of a region over which the dependent variable (in this case, pressure) is governed by a parabolic partial differential equation.

There is virtually no prior available work on this problem. In one study Hari [44] used the calculus of variations and the Ritz method to determine optimum boundaries for elliptic systems. Since the

solution necessitates that the boundary functions appear explicitly in the Ritz approximation, Hari's results are of limited general utility, particularly to parabolic problems involving petroleum reservoirs. The method developed here, based on the variation of a functional on a variable region [41,61] is applicable to general parabolic systems with arbitrarily-varying physical properties subject to either Dirichlet or Neumann boundary conditions.

For reasons of economy, the time allowable for closing wells is limited. It is important, therefore, that any method developed for estimating the shape of a reservoir be applicable in the late transient period of well production. To demonstrate this point we present two computational examples to illustrate that the shape of a reservoir may be estimated on the basis of late transient data only. The first example is the estimation of the radius of a bounded circular reservoir, while the second is the estimation of the shape of a two-dimensional, single-phase reservoir with constant pressure outer boundary.

2. Formulation of the Optimum Boundary Problem

Let us consider a reservoir of uniform thickness h but of arbitrary shape and permeability distribution and containing N production wells and $M-N$ "pure" observation wells, for which the production flow rates are zero. Figure IV-1 shows schematically such a reservoir. The radius and production flow rate of the j^{th} well will be denoted by r_{ω_j} and q_j , respectively. The governing equation for the pressure in a reservoir containing a single-phase fluid can be

written

$$\frac{\partial p}{\partial t} = \nabla(\alpha(\underline{r})\nabla p) \quad \underline{r} \in S \quad (1)$$

where $\alpha(\underline{r}) = k(\underline{r})/\phi\mu c$ is the hydraulic diffusivity, ∇ is the two-dimensional gradient operator with respect to the position vector $\underline{r} = (x,y)$, and S is the extent of the region in the two-dimensional plane (unknown). Boundary conditions are given on the boundaries B_{ω_j} of each well and on the external boundary of the reservoir B_e as follows:

$$\underline{r} \in B_{\omega_j} \quad \frac{\partial p}{\partial \ell} = 0 \quad j=1, \dots, M \quad (2)$$

$$h \int_{B_{\omega_j}} \frac{k(\underline{r})}{\mu} \frac{\partial p}{\partial n} d\ell = \begin{cases} q_j & j=1, 2, \dots, N \\ 0 & j=N+1, \dots, M \end{cases} \quad (3)$$

$$\underline{r} \in B_e \quad p(\underline{r}, t) = p(\underline{r}, 0) \quad (4)$$

$$\text{or} \quad \frac{\partial p}{\partial n} = 0 \quad (5)$$

where $\frac{\partial p}{\partial n}$ and $\frac{\partial p}{\partial \ell}$ are the normal and tangential derivatives to the indicated boundary, either B_{ω_j} or B_e . Equation (2) specifies that the pressure on the periphery of the j^{th} well is uniform, while Eq. (3) specifies the production rate in terms of an integral of the flux. Equations (4) and (5) express the two commonly employed boundary conditions at the boundary of a reservoir, either constant pressure or impermeability. Note that we choose the outwardly directed normal to the boundary as positive. The initial condition to Eq. (1) can be

taken as some specified pressure distribution

$$p(\underline{r}, 0) = p_0(\underline{r}) \quad (6)$$

Say the reservoir contains M observation wells at coordinate locations $\underline{r}_1, \underline{r}_2, \dots, \underline{r}_N, \underline{r}_{N+1}, \dots, \underline{r}_M$. Without loss of generality, we number the wells such that the first N wells (out of M total wells) are the production wells. The observed pressures at each of the M wells will be denoted by $p^{\text{obs}}(\underline{r}_j, t)$. The problem is to determine the location of the outer boundary of the reservoir B_e such that an objective function related to the discrepancy between predicted and observed pressures is minimized. A common form of such a function is the sum of squares

$$J = \int_0^T \sum_{j=1}^M Q_j [p^{\text{obs}}(\underline{r}_j, t) - p(\underline{r}_j, t)]^2 dt \quad (7)$$

where T is the total time period over which observations are available, Q_j is an arbitrary positive weighting factor, $p^{\text{obs}}(\underline{r}_j, t)$ and $p(\underline{r}_j, t)$ are the observed and predicted pressures at the j^{th} well which is at location \underline{r}_j , $j=1, 2, \dots, M$. For the case of measurements made at discrete times the objective function can be defined as follows. If we have n_1 measurements at well 1 at n_1 different times, n_2 measurements at well 2 at n_2 different times, \dots , and n_M measurements at well M at n_M different times, we define the objective function as

$$J = \sum_{j=1}^M \sum_{i=1}^{n_j} Q_j [p^{\text{obs}}(\underline{r}_j, t_i) - p(\underline{r}_j, t_i)]^2 \quad (8)$$

This objective function can be placed in the form of Eq. (7) as follows

$$J = \int_0^T \sum_{j=1}^M \sum_{i=1}^{n_j} Q_j [p^{\text{obs}}(\tilde{r}_j, t) - p(\tilde{r}_j, t)]^2 \delta(t-t_i) dt \quad (9)$$

where $\delta(\cdot)$ is the Dirac delta function.

Since Eq. (8) can be written in the form of Eq. (7), we shall henceforth take Eq. (7) as the general objective function which we desire to minimize.

Because of the uniformity of pressure around the circumference of the wells, i.e., Eq. (2), Eq. (7) can be written as

$$J = \sum_{j=1}^M \frac{Q_j}{2\pi r_{\omega_j}} \int_0^T \int_{B_{\omega_j}} [p^{\text{obs}}(\tilde{r}, t) - p(\tilde{r}, t)]^2 d\ell dt \quad (10)$$

Summarizing, we wish to minimize J subject to Eqs. (1)-(3), Eq. (4) or (5), and Eq. (6), by determining the location of the boundary B_e , that is, we wish to determine the coordinate location of each point of B_e , a closed region in the x - y plane. As such, this problem can be viewed as an optimal control problem in which the location of the boundary is the control variable. Such problems, involving systems governed by partial differential equations have not heretofore been solved. Thus, although the solution we present in the next section is directed toward the specific reservoir boundary problem, it is, in fact, generally applicable to optimum boundary problems in distributed parameter systems.

3. Derivation of the Solution of the Optimum Boundary Problem

As we have just noted, the minimization of J subject to Eqs. (1)-(6) by choice of the coordinate location of each point of the boundary B_e constitutes an optimal control problem in which the boundary location is the control variable. Optimal control problems of this complexity do not possess analytical solutions, and by application of the maximum principle for distributed parameter systems [78], the solution of these types of problems reduces to two-point boundary value problems in a function space. Such two-point boundary value problems must be solved iteratively. Consequently, we develop in this section a solution by a method of steepest descent, wherein an initial guess of the boundary location is iteratively improved such that J is continually decreased. In this form the algorithm is similar in nature to that proposed in Chapter III for the estimation of spatially-varying reservoir properties from well-pressure data.

Our derivation is based on the variation of a functional on a variable region. In particular, we wish to relate a perturbation in the boundary position δB_e to a perturbation in the objective function J , δJ . By so doing we can then choose δB_e in such a way that $\delta J < 0$ and, consequently, such that each iteration serves to decrease J .

We begin by transforming the constrained optimal control problem into an unconstrained problem through the introduction of adjoint variables. We redefine the objective function by

$$J_\lambda = J + \int_0^T \int_S \lambda(\underline{r}, t) \left[\nabla(\alpha(\underline{r}) \nabla p) - \frac{\partial p}{\partial t} \right] ds dt \quad (11)$$

where $\lambda(\underline{r}, t)$ is the adjoint variable. Then if B_e^* is the optimal reservoir boundary which minimizes J , it also clearly minimizes J_λ .

Assume the outer boundary is perturbed from B_e to $B_e + \delta B_e$ with a consequent mapping of the domain S into $S + \delta S$, the domain corresponding to $B_e + \delta B_e$. The perturbation in B_e introduces a perturbation in J_λ . Then the first variation of J_λ contains two terms, one due to the variation of the integrand and the other due to the variation of the domain of integration

$$\begin{aligned} \delta J_\lambda = & \sum_{j=1}^M \frac{Q_j}{2\pi r_{\omega_j}} \int_0^T \int_{B_{\omega_j}} [p^{\text{obs}}(\underline{r}, t) - p^*(\underline{r}, t)]^2 d\ell dt \\ & - \sum_{j=1}^M \frac{Q_j}{2\pi r_{\omega_j}} \int_0^T \int_{B_{\omega_j}} [p^{\text{obs}}(\underline{r}, t) - p(\underline{r}, t)]^2 d\ell dt \\ & + \int_0^T \int_S \lambda(\underline{r}, t) \left[\nabla(\alpha(\underline{r}) \nabla p^*(\underline{r}, t)) - \frac{\partial p^*(\underline{r}, t)}{\partial t} \right] ds dt \\ & - \int_0^T \int_S \lambda(\underline{r}, t) \left[\nabla(\alpha(\underline{r}) \nabla p(\underline{r}, t)) - \frac{\partial p(\underline{r}, t)}{\partial t} \right] ds dt \\ & + \int_0^T \int_{\delta S} \lambda(\underline{r}, t) \left[\nabla(\alpha(\underline{r}) \nabla p^*(\underline{r}, t)) - \frac{\partial p^*(\underline{r}, t)}{\partial t} \right] ds dt \end{aligned} \quad (12)$$

where $p(\underline{r}, t)$ is the solution with the boundary B_e and $p^*(\underline{r}, t)$ is the solution with the new boundary $B_e^* = B_e + \delta B_e$. In writing Eq.

(12) we have implicitly assumed that all wells at which data are available are within the same reservoir. This means that all data wells are within the boundary to be estimated. (In order to assure that all data wells lie in the same reservoir one might make well interference tests in advance.)

We note that no matter how the boundary changes, the pressure still satisfies Eq. (1). Thus, Eq. (12) can be written as

$$\begin{aligned}
 \delta J_{\lambda} = & \sum_{j=1}^M \frac{Q_j}{2\pi r_{\omega_j}} \int_0^T \int_{B_{\omega_j}} [p^{\text{obs}}(\underline{r},t) - p^*(\underline{r},t)]^2 d\ell dt \\
 & - \sum_{j=1}^M \frac{Q_j}{2\pi r_{\omega_j}} \int_0^T \int_{B_{\omega_j}} [p^{\text{obs}}(\underline{r},t) - p(\underline{r},t)]^2 d\ell dt \\
 & + \int_0^T \int_S \int \lambda(\underline{r},t) [\nabla(\alpha(\underline{r}) \nabla p^*(\underline{r},t)) - \frac{\partial p^*(\underline{r},t)}{\partial t}] ds dt \\
 & - \int_0^T \int_S \int \lambda(\underline{r},t) [\nabla(\alpha(\underline{r}) \nabla p(\underline{r},t)) - \frac{\partial p(\underline{r},t)}{\partial t}] ds dt \quad (13)
 \end{aligned}$$

We expand the integrand of the first term on the right-hand side of Eq. (13) in a Taylor series with respect to $p(\underline{r},t)$ and retain only the first order term. Then Eq. (13) becomes

$$\begin{aligned}
 \delta J_{\lambda} = & \sum_{j=1}^M \frac{Q_j}{2\pi r_{\omega_j}} \int_0^T \int_{B_{\omega_j}} -2[p^{\text{obs}}(\underline{r},t) - p(\underline{r},t)]\delta p(\underline{r},t) d\ell dt \\
 & + \int_0^T \int_S \int \lambda(\underline{r},t) [\nabla(\alpha(\underline{r}) \nabla \delta p(\underline{r},t)) - \frac{\partial \delta p(\underline{r},t)}{\partial t}] ds dt \quad (14)
 \end{aligned}$$

where $\delta p(\underline{r}, t) = p^*(\underline{r}, t) - p(\underline{r}, t)$.

Using the identity

$$\begin{aligned} \lambda \nabla(\alpha(\underline{r}) \nabla \delta p) &\equiv \nabla(\lambda \alpha(\underline{r}) \nabla \delta p) - (\nabla \lambda) \cdot \alpha(\underline{r}) \nabla \delta p \\ &\equiv \nabla(\lambda \alpha(\underline{r}) \nabla \delta p) - \nabla \delta p \cdot (\alpha(\underline{r}) \nabla \lambda) \\ &\equiv \nabla(\lambda \alpha(\underline{r}) \nabla \delta p) - \nabla(\delta p \alpha(\underline{r}) \nabla \lambda) + \delta p (\nabla(\alpha(\underline{r}) \nabla \lambda)) \end{aligned} \quad (15)$$

and $\lambda \frac{\partial \delta p}{\partial t} = \frac{\partial \lambda \delta p}{\partial t} - \frac{\partial \lambda}{\partial t} \delta p$, Eq. (14) can be expressed as

$$\begin{aligned} \delta J_\lambda &= \sum_{j=1}^M \frac{Q_j}{2\pi r_{\omega_j}} \int_0^T \int_{B_{\omega_j}} -2[p^{obs}(\underline{r}, t) - p(\underline{r}, t)] \delta p(\underline{r}, t) d\ell dt \\ &+ \int_0^T \int_S \left\{ \nabla(\lambda \alpha(\underline{r}) \nabla \delta p) - \nabla(\delta p \alpha(\underline{r}) \nabla \lambda) + \delta p \nabla(\alpha(\underline{r}) \nabla \lambda) \right. \\ &\quad \left. + \frac{\partial \lambda}{\partial t} \delta p - \frac{\partial \lambda \delta p}{\partial t} \right\} ds dt \end{aligned} \quad (16)$$

Noting that $\delta p(\underline{r}, 0) \equiv p^*(\underline{r}, 0) - p(\underline{r}, 0) = 0$, we obtain

$$\begin{aligned} \delta J_\lambda + \int_S \int \lambda \delta p(\underline{r}, t) \Big|_{t=T} ds &= \sum_{j=1}^M \frac{Q_j}{2\pi r_j} \\ &\times \int_0^T \int_{B_{\omega_j}} -2[p^{obs}(\underline{r}, t) - p(\underline{r}, t)] \delta p(\underline{r}, t) d\ell dt \\ &+ \int_0^T \int_S \left[\frac{\partial \lambda}{\partial t} + \nabla(\alpha(\underline{r}) \nabla \lambda) \right] \delta p(\underline{r}, t) ds dt \end{aligned}$$

$$+ \int_0^T \int_S [V(\lambda \alpha(\underline{r}) \nabla \delta p) - V(\delta p \alpha(\underline{r}) \nabla \lambda)] ds dt \quad (17)$$

Employing the divergence theorem, we obtain

$$\begin{aligned} \delta J_\lambda + \int_S \lambda \delta p(\underline{r}, t) \Big|_{t=T} ds &= \int_0^T \int_S [\frac{\partial \lambda}{\partial t} + \nabla(\alpha(\underline{r}) \nabla \lambda)] \delta p ds dt \\ + \sum_{j=1}^M \int_0^T \left\{ \int_{B_{\omega_j}} [\alpha(\underline{r}) \frac{\partial \lambda}{\partial n} - \frac{Q_j}{\pi r_{\omega_j}} (p^{obs}(\underline{r}, t) - p(\underline{r}, t))] d\ell \right\} \delta p dt \\ - \sum_{j=1}^M \int_0^T \int_{B_{\omega_j}} \lambda \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} d\ell dt + \int_0^T \int_{B_e} \lambda \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} d\ell dt \\ - \int_0^T \int_{B_e} (\alpha(\underline{r}) \frac{\partial \lambda}{\partial n}) \delta p d\ell dt \end{aligned} \quad (18)$$

where we have used the fact that the pressure is uniform around the periphery of each well.

Now let the adjoint variable $\lambda(\underline{r}, t)$ be governed by

$$\frac{\partial \lambda(\underline{r}, t)}{\partial t} = -\nabla(\alpha(\underline{r}) \nabla \lambda(\underline{r}, t)) \quad (19)$$

subject to the final condition

$$\lambda(\underline{r}, T) = 0 \quad (20)$$

The choice of the boundary conditions for Eq. (19) will depend on the type of the boundary conditions at the outer boundary for Eq. (1). Two

types of boundary conditions, namely, constant pressure, Eq. (4), and no flow, Eq. (5), will be treated as follows:

(a) Constant pressure along the outer boundary

In this case the boundary conditions for Eq. (19) are chosen such that the second, third, and fourth terms on the right-hand side of Eq. (18) vanish. This can be done as follows. Because of the arbitrariness of $\frac{\partial \delta p}{\partial n}$ on the outer boundary and the arbitrariness and uniformity of δp on the inner boundaries, B_{ω_j} , $j=1, \dots, M$,

$$\sum_{j=1}^M \int_0^T \left\{ \int_{B_{\omega_j}} \left[\alpha(\underline{r}) \frac{\partial \lambda}{\partial n} - \frac{Q_j}{\pi r_{\omega_j}} (p^{obs}(\underline{r}, t) - p(\underline{r}, t)) \right] d\ell \right\} \delta p dt = 0$$

and

$$\int_0^T \int_{B_e} \lambda \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} d\ell = 0$$

imply

$$\int_{B_{\omega_j}} \alpha(\underline{r}) \frac{\partial \lambda}{\partial n} d\ell = 2Q_j [p^{obs}(\underline{r}, t) - p(\underline{r}, t)] \quad \underline{r} \in B_{\omega_j}, j=1, \dots, M \quad (21)$$

and

$$\lambda(\underline{r}, t) = 0 \quad \underline{r} \in B_e \quad (22)$$

respectively. To find the third boundary condition, we note that from Eq. (3)

$$\int_{B_{\omega_j}} \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} d\ell = 0 \quad \underline{r} \in B_{\omega_j}, j=1, \dots, M$$

and that in order for the relation

$$\sum_{j=1}^M \int_0^T \int_{B_{\omega_j}} \lambda \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} d\ell dt = 0$$

to hold, a necessary and sufficient condition is that [31]

$$\frac{\partial \lambda(\underline{r}, t)}{\partial \ell} = 0 \quad \underline{r} \in B_{\omega_j}, j=1, \dots, M \quad (23)$$

This is the third boundary condition.

Substituting Eqs. (19)-(23) into Eq. (18) we obtain

$$\delta J_{\lambda} = - \int_0^T \int_{B_e} \alpha(\underline{r}) \frac{\partial \lambda}{\partial n} \delta p d\ell dt \quad (24)$$

In order to use the fact that the boundary condition for the unperturbed and perturbed boundaries should be the same, i.e., $p^*(\underline{R} + \delta \underline{R}(\underline{r})) = p(\underline{R}) = p_0(\underline{R})$ where \underline{R} is a point on B_e and $\underline{R} + \delta \underline{R}(\underline{r})$ which corresponds to \underline{R} under perturbation is a point on $B_e + \delta B_e$. As shown in Figure IV-2, we express δp as

$$\begin{aligned}
 \delta p(\underline{R}, t) &\equiv p^*(\underline{R}, t) - p(\underline{R}, t) \\
 &\approx p^*(\underline{R} + \delta \underline{R}(\underline{r})) + \left(\frac{\partial p^*(\underline{R} + \delta \underline{R}(\underline{r}))}{\partial \underline{r}} \right)^T (\underline{R} - \underline{R} - \delta \underline{R}(\underline{r})) - p(\underline{R}) \\
 &= - \left(\frac{\partial p^*(\underline{R} + \delta \underline{R}(\underline{r}))}{\partial \underline{r}} \right)^T \delta \underline{R}(\underline{r})
 \end{aligned}
 \tag{25}$$

where superscript T denotes the transpose of the quantity.

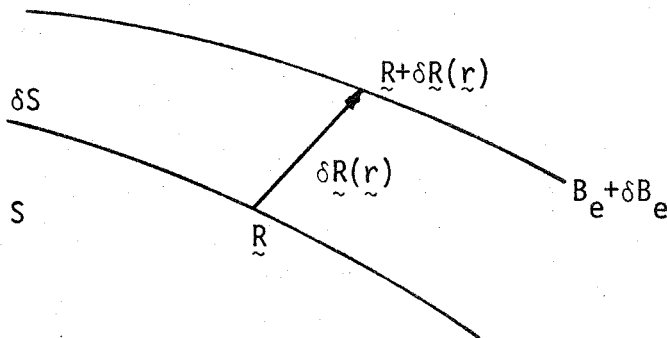


Figure IV-2

Note that $\delta \underline{R}(\underline{r})$ is a function of position along the unperturbed boundary. Since $\frac{\partial p(\underline{R})}{\partial \underline{r}}$ and $\frac{\partial p^*(\underline{R} + \delta \underline{R})}{\partial \underline{r}}$ differ only by a quantity of order $\delta \underline{R}$, Eq. (25) becomes

$$\delta p(\underline{R}, t) = - \left(\frac{\partial p(\underline{R}, t)}{\partial \underline{r}} \right)^T \delta \underline{R}(\underline{r})
 \tag{26}$$

Substituting Eq. (26) into Eq. (24) yields

$$\delta J_\lambda = \int_0^T \int_{B_e} \alpha(\underline{r}) \frac{\partial \lambda}{\partial n} \left(\frac{\partial p}{\partial \underline{r}} \right)^T \delta \underline{R}(\underline{r}) \, d\ell \, dt \quad (27)$$

Changing the order of integration, we have

$$\delta J_\lambda = \int_{B_e} \left[\int_0^T \alpha(\underline{r}) \frac{\partial \lambda}{\partial n} \left(\frac{\partial p}{\partial \underline{r}} \right)^T \, dt \right] \delta \underline{R}(\underline{r}) \, d\ell \quad (28)$$

At this point we note that the perturbation in the boundary location δB_e has been replaced by $\delta \underline{R}(\underline{r})$, the vector difference in the boundary coordinates at each position along the original boundary. In the iterative, steepest descent solution of the problem we wish to choose $\delta \underline{R}(\underline{r})$ at each iteration such that J_λ is decreased. We compute $\delta \underline{R}(\underline{r})$ by

$$\delta \underline{R}(\underline{r}) = -W(\underline{r}) \left[\int_0^T \alpha(\underline{r}) \frac{\partial \lambda}{\partial n} \left(\frac{\partial p}{\partial \underline{r}} \right)^T \, dt \right]^T \quad \underline{r} \in B_e \quad (29)$$

where $W(\underline{r})$ is an arbitrary positive weighting function of \underline{r} .

(b) No flow across the exterior boundary

In this case the boundary conditions for Eq. (19) are chosen such that the second, third, and fifth terms on the right-hand side of Eq. (18) vanish. As with the arguments given in the case of (a), Eqs. (21) and (23) are also the boundary conditions for this case. Because of the arbitrariness of δp on the exterior boundary

$$\int_0^T \int_{B_e} (\alpha(\underline{r}) \frac{\partial \lambda}{\partial n}) \delta p \, d\ell \, dt = 0$$

implies

$$\frac{\partial \lambda(\underline{r}, t)}{\partial n} = 0 \quad \underline{r} \in B_e \quad (30)$$

This is the third boundary condition for this case. Using Eqs. (19), (20), (21), (23) and (30), Eqs. (18) becomes

$$\delta J_\lambda = \int_0^T \int_{B_e} \lambda \alpha(\underline{r}) \frac{\partial \delta p}{\partial n} \, d\ell \, dt \quad (31)$$

Since $\delta p \equiv p^*(\underline{r}, t) - p(\underline{r}, t)$ and $\frac{\partial p(\underline{r}, t)}{\partial n} = 0$ along B_e , Eq. (31) can be written as

$$\delta J_\lambda = \int_0^T \int_{B_e} \lambda \alpha(\underline{r}) \frac{\partial p^*(\underline{r}, t)}{\partial n} \, d\ell \, dt \quad (32)$$

In order to be able to use the iterative method $\frac{\partial p^*(\underline{r}, t)}{\partial n}$ should be approximated by $\frac{\partial p(\underline{r}, t)}{\partial n}$. This can be achieved as follows. Since the angle between n and n^* is small, it can be shown that

$$\frac{\partial p^*(\underline{R}, t)}{\partial n} = \frac{\partial p^*(\underline{R} + \delta \underline{R}, t)}{\partial n^*} - \frac{\partial^2 p(\underline{R}, t)}{\partial n^2} \delta n - \frac{\partial^2 p(\underline{R}, t)}{\partial n \partial \ell} \delta \ell \quad (33)$$

where \underline{R} is a point on B_e , $\underline{R} + \delta \underline{R}$ is a point on $B_e + \delta B_e$, n is the normal direction to B_e at the point \underline{R} , ℓ is the tangential direction to B_e at the point \underline{R} , n^* is the normal direction to the perturbed boundary $B_e + \delta B_e$ at the point $\underline{R} + \delta \underline{R}$ which corresponds to the

point \tilde{R} on B_e under perturbation, and δn and $\delta \ell$ are the normal component and tangential component of $\delta \tilde{R}$, respectively (see Figure IV-3).

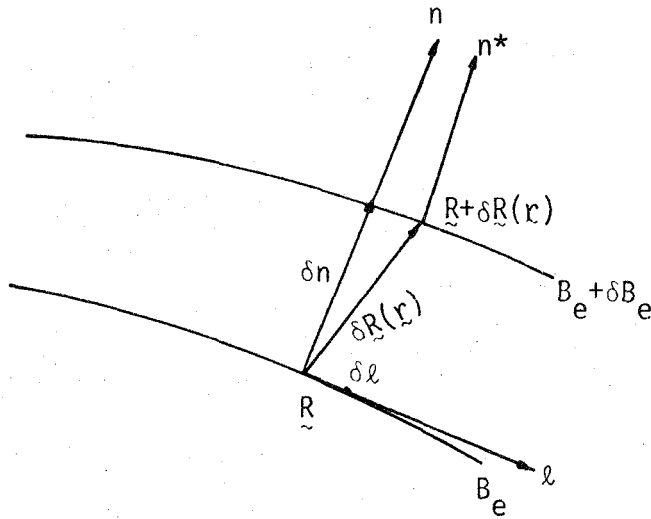


Figure IV-3

Note that δn and $\delta \ell$ are functions of position along the unperturbed boundary. Since $\frac{\partial p^*(R+\delta R, t)}{\partial n^*} = 0$, Eq. (33) becomes

$$\frac{\partial p^*(R, t)}{\partial n} = - \frac{\partial^2 p(R, t)}{\partial n^2} \delta n - \frac{\partial^2 p(R, t)}{\partial n \partial \ell} \delta \ell \quad (34)$$

Substituting Eq. (34) into Eq. (32) results in

$$\delta J = - \int_0^T \int_{B_e} [\lambda \alpha(\tilde{r}) \frac{\partial^2 p(r, t)}{\partial n^2} \delta n + \lambda \alpha(\tilde{r}) \frac{\partial^2 p(r, t)}{\partial n \partial \ell} \delta \ell] d\ell dt \quad (35)$$

At this point we note that the perturbation in the boundary location δB_e has been replaced by $\delta n(\underline{r})$ and $\delta \ell(\underline{r})$, the normal and tangential differences in the boundary coordinates at each position along the original boundary. Using the same argument as in case (a), we choose the perturbations in the normal and tangential directions as

$$\delta n = W_1(\underline{r}) \int_0^T \lambda \alpha(\underline{r}) \frac{\partial^2 p(\underline{r}, t)}{\partial n^2} dt \quad \underline{r} \in B_e \quad (36)$$

and

$$\delta \ell = W_2(\underline{r}) \int_0^T \lambda \alpha(\underline{r}) \frac{\partial^2 p(\underline{r}, t)}{\partial n \partial \ell} dt \quad \underline{r} \in B_e \quad (37)$$

where $W_1(\underline{r})$ and $W_2(\underline{r})$ are arbitrary positive weighting functions of \underline{r} , and δn and $\delta \ell$ are the variation of the boundary at the point \underline{r} in the normal and tangential directions, respectively.

From the definition of the functional derivative and from Eqs. (28) and (35) we can see that we define the perturbations in order to seek the minimum of the objective function by moving the boundary along the gradient of the objective function with respect to the location of the boundary from one iteration to the next. The size of the step, i.e., how far a distance one must proceed along the gradient in each iteration, is controlled by the choice of the weighting factor W in Eq. (29) or W_1 and W_2 in Eqs. (36) and (37), respectively. One method of choosing the weighting factor is to minimize the objective function along the direction of the gradient with respect to the weighting factor, generally necessitating a one-dimensional search. The step size can also be determined from the second variation of the

objective function. In the former method, we are required to solve the state equation several times. In the latter method, the calculation of the second variation of J is needed. As pointed out previously, a considerable portion of computational time in each iteration in the parameter estimation is devoted to the determination of the solutions of the state and the adjoint equations. Although the determination of the weighting factor by the optimization procedures usually reduces the number of total iterations, the computational efforts can be considerable. Thus, in this study, the weighting factor is chosen for the first iteration such that the perturbation will be some percentage of the initial guess value of the parameter (say 30%). If the new estimate increases rather than decreases the objective function, the minimum has been overstepped. We then go back to the value from the previous iteration and decrease the weighting factor by a factor of two before forming the new estimate. If the new estimate decreases the objective function, the value of the weighting factor is tripled for the next iteration.

In order to increase the rate of convergence, a more effective gradient method, such as the conjugate gradient method, may be employed instead of steepest descent. However, in using that method a one-dimensional search technique is required to determine the size of the step. Whether or not this can reduce the overall computational time for complicated systems is not clear a priori. Future work is necessary to determine whether or not it is advantageous to employ

auxiliary routines to optimize the step length taken in the gradient direction in history-matching algorithms based on optimal control theory.

In summary, the algorithm is used as follows:

1. Make an initial guess for the location of the boundary B_e^0 and solve Eqs. (1)-(6). Evaluate J by Eq. (7).
2. Compute $\lambda(r,t)$ by solving Eqs. (19)-(23) from $t = T$ to $t = 0$ for the case of constant pressure on the outer boundary, or by solving Eqs. (19), (20), (21), (23), and (30) from $t = T$ to $t = 0$ for the case of no flow across the outer boundary.
3. Compute $\delta R(r)$ by Eq. (29) for the case of constant pressure on the exterior boundary or by Eqs. (36) and (37) for the case of no flow across the outer boundary and up-date the boundary by

$$B_e^{j+1} = B_e^j + \delta B_e$$

4. If a convergence criterion

$$\frac{J^j - J^{j+1}}{J^j} \leq \epsilon$$

is met, stop; if not, return to step 1 with B_e^{j+1} in place of B_e^0 .

In the next section we present a detailed application of the algorithm to the estimation of the location of the boundary for a one-dimensional and a two-dimensional hypothetical single-phase

reservoir.

4. Examples

4.1 Example 1: Estimation of the Location of the Boundary for a One-Dimensional, One-Phase, Bounded Reservoir

We consider the estimation of the location of the boundary for a one-dimensional, one-phase, bounded reservoir, i.e., a circular reservoir with a centrally-located producing well. The reservoir pressure is governed by

$$\frac{\partial p(x,t)}{\partial t} = \frac{k}{\alpha} e^{-2mx} \frac{\partial^2 p(x,t)}{\partial x^2} \quad \begin{array}{l} 0 < t \leq T \\ 0 < x < 1 \end{array} \quad (38)$$

$$p(x,0) = p_0(x) \quad (39)$$

$$\frac{\partial p}{\partial x} = \frac{\beta q}{k} \quad x = 0 \quad (40)$$

$$\frac{\partial p}{\partial x} = 0 \quad x = 1 \quad (41)$$

where $x = [\ln(r/r_w)]/m$, $m = \ln(r_e/r_w)$, $\alpha = \phi \mu c m^2 r_w^2$, $\beta = \mu m / 2\pi h$, r_w is the radius of the well, and r_e is the radius of the reservoir. The true but unknown radius of the reservoir will be taken to be $r_e = 50$ ft. "Observed pressures" at the well were generated by adding normally distributed random error with mean zero and standard deviation $\sigma = 0.0, 0.2,$ and 1.0 psi to the numerical solution of

Eqs. (38)-(41) with the following parameter values: $\phi = 0.1$, $h = 10$ ft, $r_w = 0.25$ ft, $k = 20$ md, $c = 10^{-5}$ psi $^{-1}$, $\mu = 1$ cp, $p_o(x) = 4000$ psi, and $q = 100$ bbl/day. Data were recorded at increments of 0.1 min. The initial guess of r_e for use in the estimation algorithm is 100 ft.

The adjoint equations for this system are

$$\frac{\partial \lambda}{\partial t} = -\frac{k}{\alpha} \frac{\partial^2}{\partial x^2} (\lambda e^{-2mx}) \quad (42)$$

$$\lambda(x, T) = 0 \quad (43)$$

$$\frac{\partial \lambda}{\partial x} = 2m\lambda + \frac{2\alpha}{k} [p^{obs}(x, t) - p(x, t)] \quad x = 0 \quad (44)$$

$$\frac{\partial \lambda}{\partial x} = 2m\lambda \quad x = 1 \quad (45)$$

The correction for each iteration is given by

$$\delta x \Big|_{x=1} = W \frac{k}{\alpha} e^{-2m} \int_0^T \lambda u_{xx} \Big|_{x=1} dt \quad (46)$$

Figure IV-4 presents the estimated value of r_e as functions of T , the time period over which observations are available and σ , the error standard deviation. The points t_* and t^* separate the data in the transient, late transient, and semi-steady periods. The times t_* and t^* are defined by Matthews and Russell [58] as $t_* \cong \phi \mu c r_e^2 / 0.00264K$ and $t^* \cong \phi \mu c r_e^2 / 0.00088K$, in practical units. At

the lower error, $\sigma = 0.0$ and $\sigma = 0.2$, the estimate is insensitive to the value of T . At the higher error, $\sigma = 1.0$, the estimate is relatively sensitive to the value of T when T is within the late transient period. However, even in the case of $\sigma = 1.0$ the error in the estimated value of the reservoir radius is only about four percent. Thus we can conclude that this method is capable of estimating the location of the boundary using the data in the late transient period for a radial reservoir with a centrally-located well. Figure IV-5 shows the actual and estimated pressures. The pressures associated with the true and estimated radii are too close to plot as separate curves. From this figure we can see that we are not able to obtain an accurate estimate by using the data solely in the early transient period since, of course, the effect of the boundary is not yet reflected at the well.

For examining the effect of the initial guess r_e^0 on the estimate of r_e , a test with $r_e^0 = 25$ ft, $\sigma = 0.2$, and $T = 20$ min was made. The results for the case of $r_e^0 = 25$ ft and the case of $r_e^0 = 100$ ft are shown in Table IV-1. We see that there is essentially no difference between the estimates \hat{r}_e for $r_e^0 = 25$ ft and $r_e^0 = 100$ ft.

Table IV-1. Effect of the Initial Guess r_e^0 on the Estimate \hat{r}_e

Initial Guess r_e^0 (ft)	σ	T(min)	Iterations	Computing Time*(sec)	Value of J Initial	Final	Estimate \hat{r}_e
100	0.2	20	9	22.45	3.24×10^4	8.52	49.972
25	0.2	20	7	20.05	3.48×10^6	8.92	49.950

* IBM 370/158

4.2 Example 2: Estimation of the Location of the Boundary for a Two-Dimensional, One-Phase Reservoir with Constant Pressure Outer Boundary

We consider the estimation of the location of the boundary for the single-phase reservoir shown in Figure IV-6, the pressure in which is governed by

$$\frac{\partial p}{\partial t} = \frac{1}{c\phi\mu} \left[\frac{\partial}{\partial x} \left(k(x,y) \frac{\partial p}{\partial x} \right) + \frac{\partial}{\partial y} \left(k(x,y) \frac{\partial p}{\partial y} \right) \right] \quad (47)$$

$$p(x,y,0) = p_0 \quad x,y \in S \quad (48)$$

$$p(x,y,t) = p \quad x,y \in B_e \quad (49)$$

$$h \int_B \frac{k}{\mu} \frac{\partial p}{\partial n} d\ell = q \quad (\text{injection well}) \quad (50)$$

$$h \int_{B_j} \frac{k}{\mu} \frac{\partial p}{\partial n} d\ell = 0 \quad (\text{observation wells}) \quad j=1,2 \quad (51)$$

The adjoint equations for this system are

$$\frac{\partial \lambda}{\partial t} = - \frac{1}{c\phi\mu} \left[\frac{\partial}{\partial x} \left(k(x,y) \frac{\partial \lambda}{\partial x} \right) + \frac{\partial}{\partial y} \left(k(x,y) \frac{\partial \lambda}{\partial y} \right) \right] \quad (52)$$

$$\lambda(x,y,T) = 0 \quad x,y \in S \quad (53)$$

$$\lambda(x,y,t) = 0 \quad x,y \in B_e \quad (54)$$

$$\int_B \frac{k(x,y)}{c\phi\mu} \frac{\partial \lambda}{\partial n} d\ell = 2[p^{\text{obs}}(x,y,t) - p(x,y,t)] \quad (\text{injection well}) \quad (55)$$

$$\int_{B_j} \frac{k(x,y)}{c\phi\mu} \frac{\partial \lambda}{\partial n} d\ell = 2[p^{obs}(x,y,t) - p(x,y,t)]$$

(observation wells) $j=1,2$ (56)

$$\frac{\partial \lambda(x,y,t)}{\partial \ell} = 0 \quad x,y \in B \quad (57)$$

$$\frac{\partial \lambda(x,y,t)}{\partial \ell} = 0 \quad x,y \in B_j \quad j=1,2 \quad (58)$$

The corrections for each iteration are given by

$$\delta x = -w(x,y) \int_0^T \frac{k(x,y)}{c\phi\mu} \frac{\partial \lambda}{\partial n} \frac{\partial p}{\partial x} dt \quad x,y \in B_e \quad (59)$$

$$\delta y = -w(x,y) \int_0^T \frac{k(x,y)}{c\phi\mu} \frac{\partial \lambda}{\partial n} \frac{\partial p}{\partial y} dt \quad x,y \in B_e \quad (60)$$

The true but unknown shape of the reservoir and the initial guess of the boundary of the reservoir are shown in Figure IV-6. The locations of the injection and observation wells are also shown in Figure IV-6. We note that the injection well also serves as an observation well. Observed pressures were generated by solving Eqs. (47)-(51) with the true shape shown in Figure IV-6 and the following parameter values: $\phi = 0.2$, $h = 1$ ft, $c = 1.72 \times 10^{-5}$ psi⁻¹, $\mu = 0.352$ cp, $k(x,y) = 200$ md, $p_o = 0$, and $q = 500$ ft³day⁻¹ (injection). Data were recorded at increments of 5 days from $t = 0$ to $t = T = 100$ days.

In this example the objective function is reduced from $J = 699.6$ to $J = 0.001$ in five iterations and 215 seconds (IBM 370/155). Figure IV-6 shows the actual and estimated (after five iterations) shapes of the reservoir. Figure IV-7 presents the initial and the actual and estimated pressures, which are too close to plot as separate curves.

An alternative approach to determining the boundary of a reservoir is to pose the problem as one of determining the permeability distribution over a region large enough to include the reservoir. Thus, treating the permeability as the unknown property, a customary history matching exercise can be carried out with the aim being the estimation of the location of sharp decreases in the permeability distribution. Such sharp changes in the distribution of permeability would serve to define the reservoir boundary (in those situations in which the reservoir boundary results from significant changes in medium permeability). It is therefore of considerable interest to compare the results obtained with the algorithm derived in this chapter with those obtained by history matching with an unknown permeability distribution and a known boundary (chosen far enough from the wells so as to include the true boundary within it.) Since the algorithm developed in this chapter is capable of computing the boundary location as a continuous function of position, a proper comparison requires that the permeability estimating algorithm also be capable of computing the permeability distribution as a continuous function of position. A method developed in Chapter III based on an

optimal control formulation of the history-matching problem enables the estimation of reservoir properties, such as permeability and porosity, as continuous functions of position. Thus, the method proposed in Chapter III will be employed in this study.

To use the approach of estimating the location of the boundary through estimation of the permeability distribution, we impose a rectangular domain over the reservoir as shown in Figure IV-8. The true but unknown shape of the reservoir and the initial guess of the boundary of the reservoir are also shown in Figure IV-8. Observed pressures were generated at one injection well and two observation wells by solving Eqs. (47)-(51) with the following parameter values: $\phi = 0.2$, $h = 1$ ft, $c = 1.72 \times 10^{-5}$ psi⁻¹, $\mu = 0.352$ cp, $k = 200$ md inside the large circle (solid line) and $k = 10$ md outside the large circle, $p_o = 0$, and $q = 500$ ft³day⁻¹ (injection). We note that the exterior boundary is now the rectangle. Data were recorded at increments of 5 days from $t = 0$ to $t = T = 100$ days. The initial guess of the permeability distribution is $k = 200$ md within the small circle (dotted line) and $k = 10$ md outside the small circle.

In this example the objective function is reduced from $J = 39.52$ to $J = 1.58$ in ten iterations and 100 seconds (IBM 370/158). Figure IV-9 presents the distribution of permeability at $y = 12,550$ ft, $25,500$ ft, and $35,700$ ft for the initial guess, the tenth iteration, and the true permeability. As seen in this figure, in some regions far away from the wells, the permeability has only a little change from its initial guess. This is due to the fact

that the sensitivity of the pressures measured at the wells with respect to the permeabilities in those regions is very small. Therefore, it is not clear where the location of the boundary is from the distribution of permeability. In addition, in the use of this alternative approach we are required to estimate the permeability over the whole domain, whereas we need to estimate only the coordinates of the boundary in the use of the new algorithm developed in this chapter. This leads to the fact that the new algorithm converges faster than the alternative approach. Thus, we can conclude that the method developed in this chapter is a better way of determining a reservoir boundary.

5. Conclusions

In this chapter the problem of estimating the location of the boundary of a petroleum reservoir was formulated and solved by the techniques of optimal control theory for systems governed by partial differential equations. It is demonstrated that the method developed here is capable of determining the shape of a hypothetical one-dimensional and a sample two-dimensional reservoir from well pressure data in the late transient period. In addition, by comparison to solving the same problem by means of estimating an unknown permeability distribution it is shown that the new algorithm represents a more efficient (and accurate) way of determining a reservoir boundary.

It is interesting to note that in two-dimensional reservoirs, if the physical properties of the system, for example, ϕ , μ , c , h , and k are independent of position, and we observe the pressure at

one or two positions, it is clear that the solution will not be unique. In order to have a unique solution (i.e., shape), data should be available at three or more wells which do not lie on a straight line.

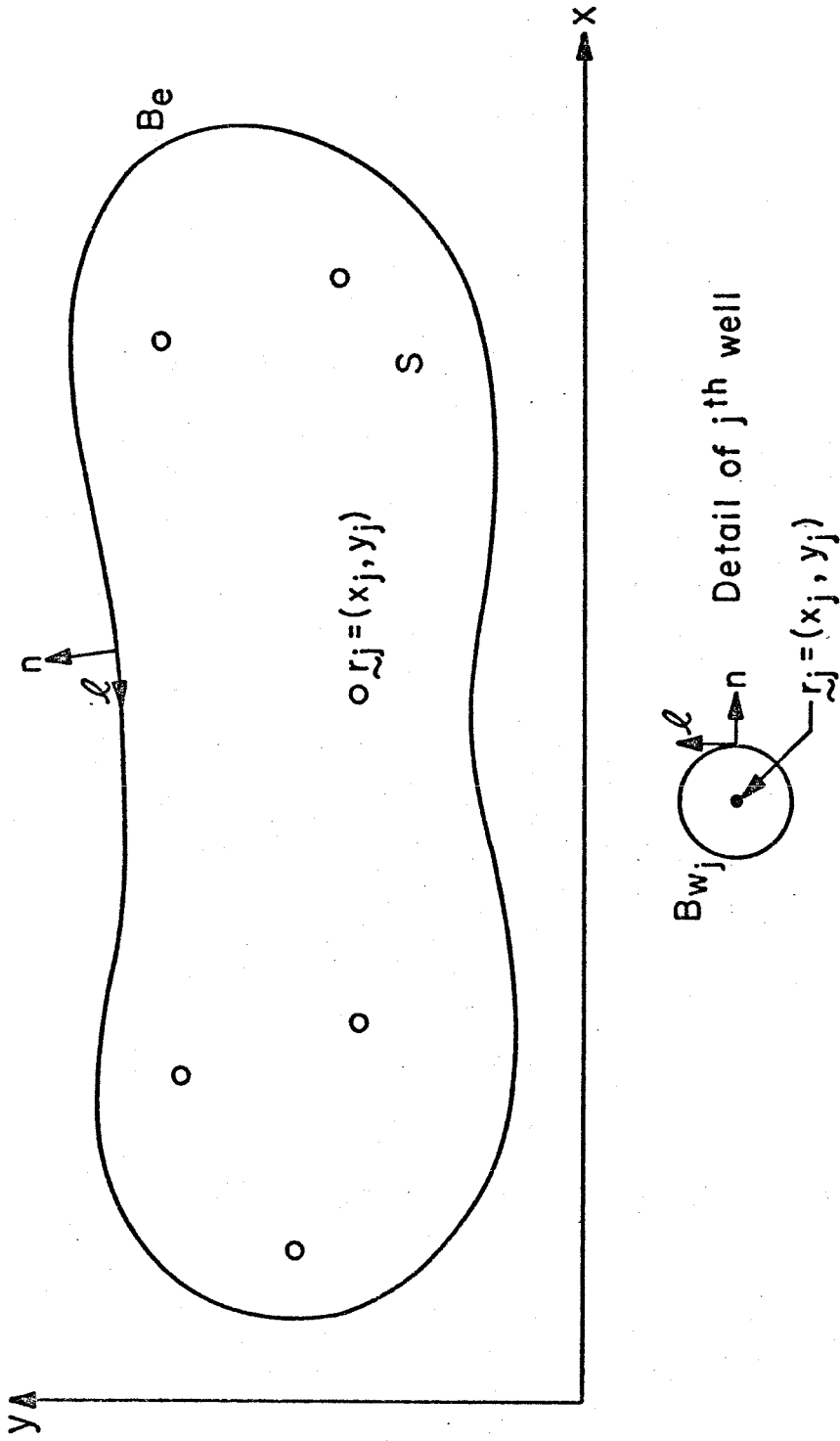


Figure IV-1. A Reservoir of General Shape

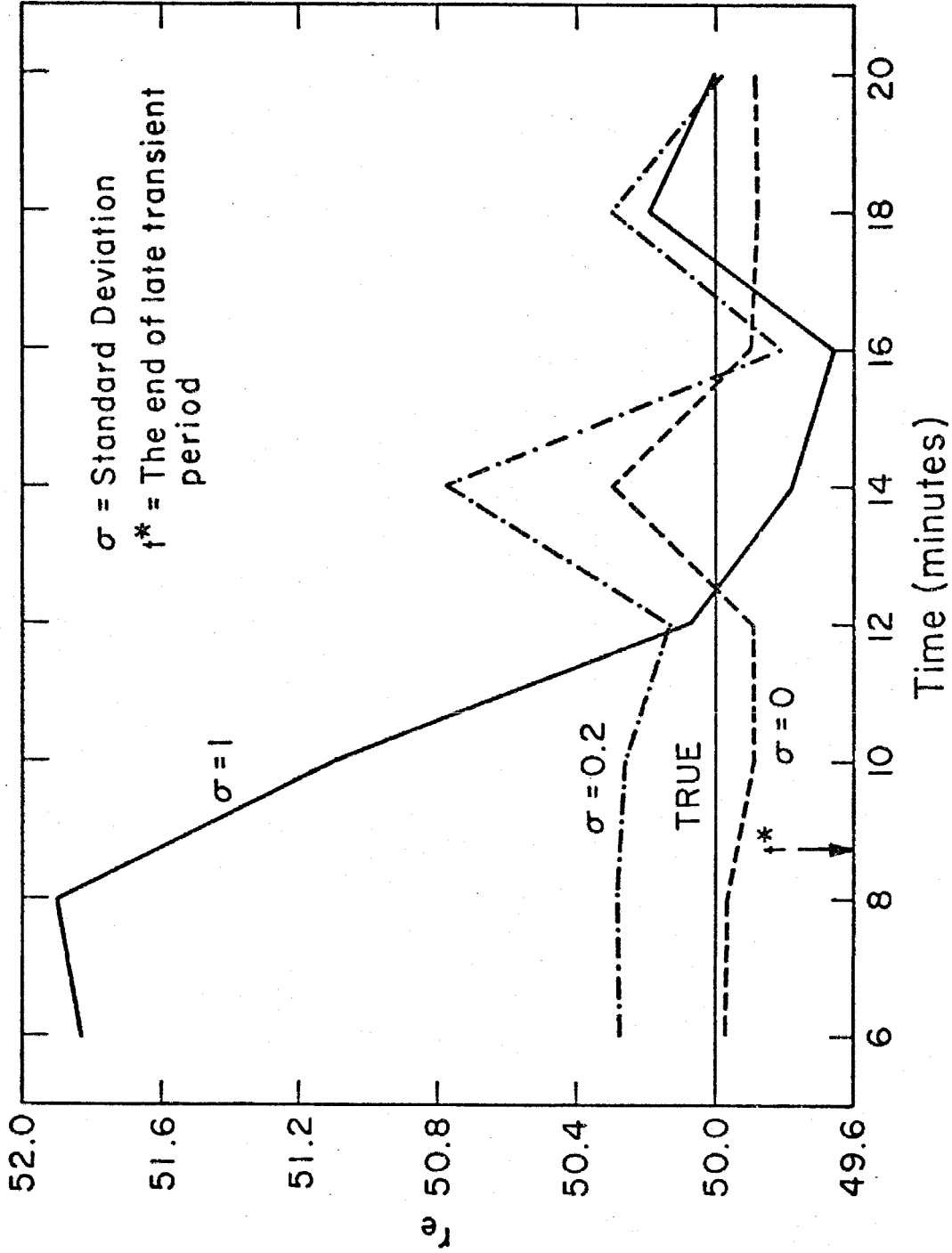


Figure IV-4. The Effect of T on the Estimation of Radius r_e

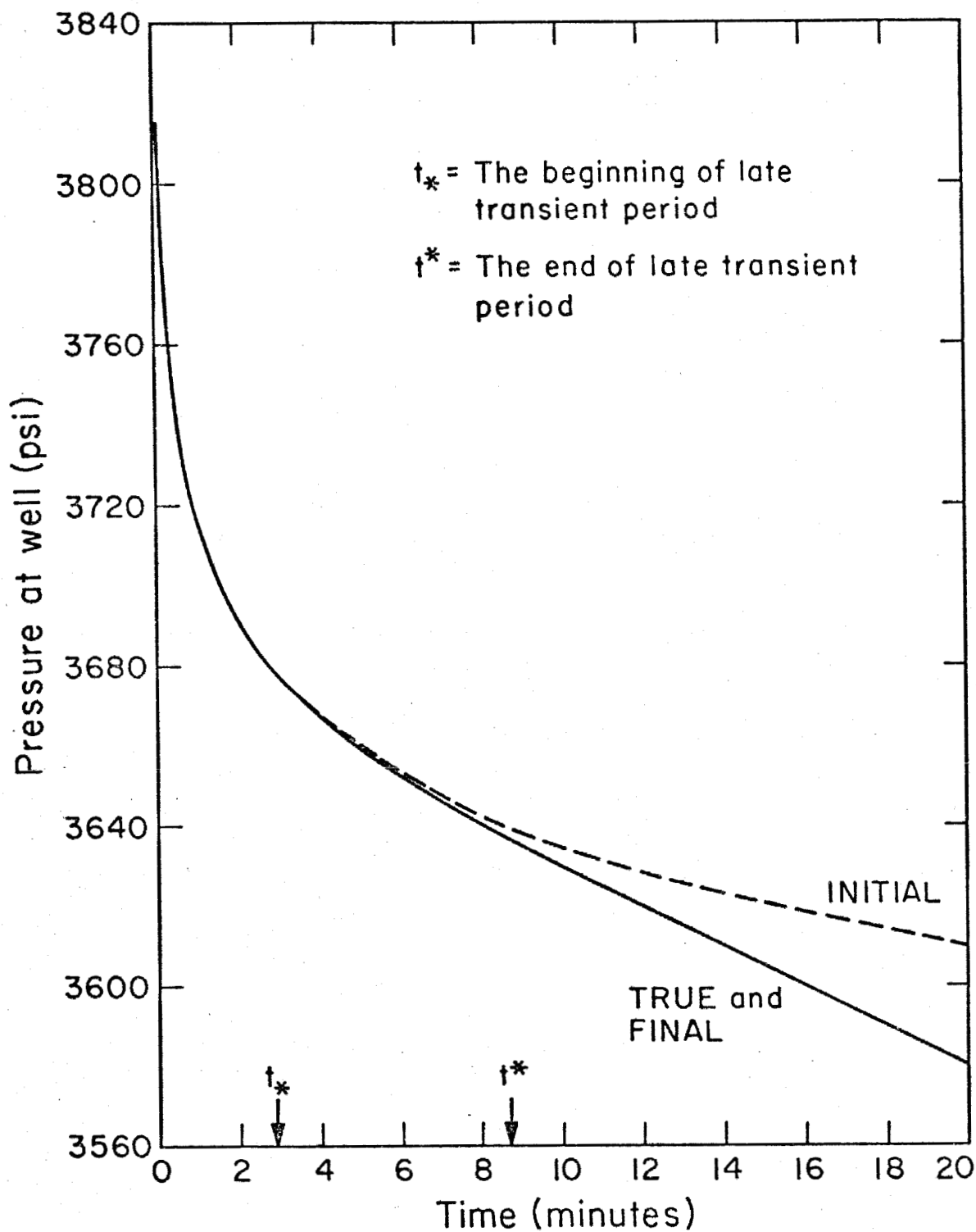


Figure IV-5. Actual and Estimated Pressure at Well

- True
- - - Initial Guess
- · - Estimate
- ↔ 5100 ft
- ⊥ Injection Well
- Observation Well

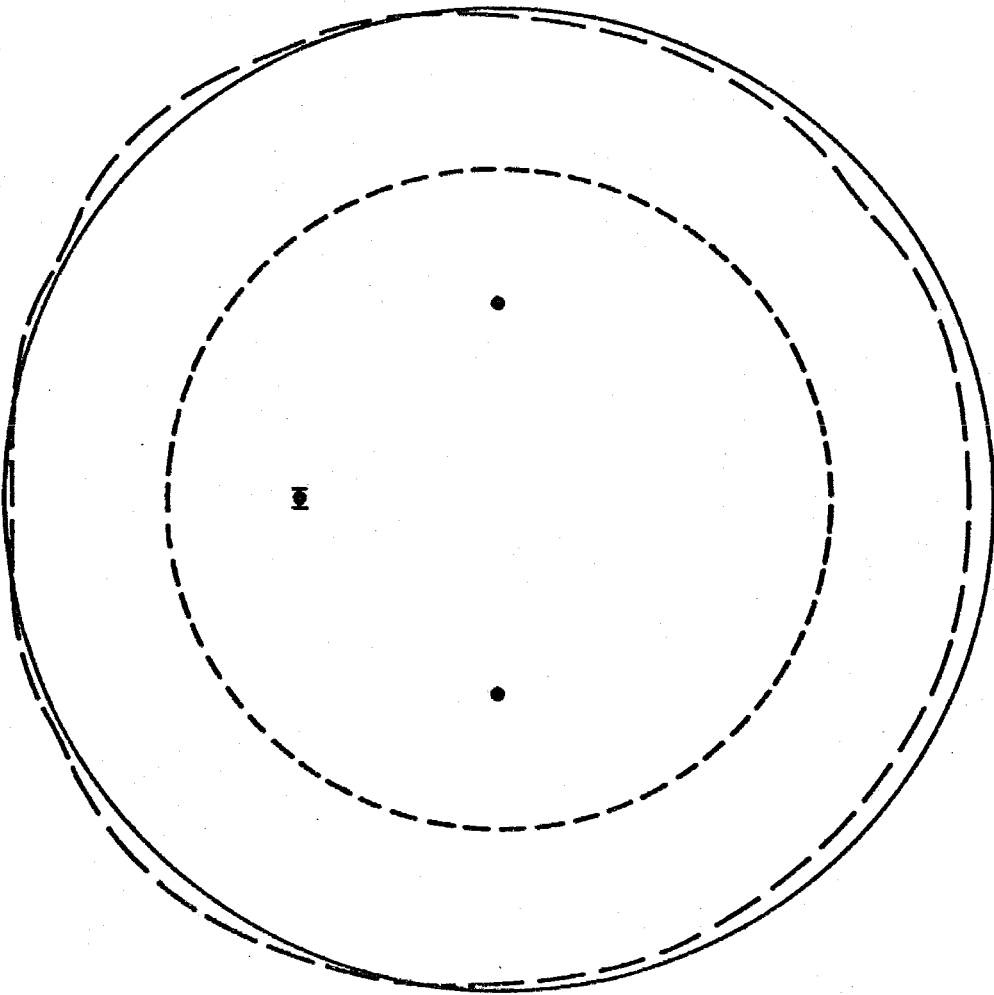


Figure IV-6. Actual and Estimated Shape of Reservoir

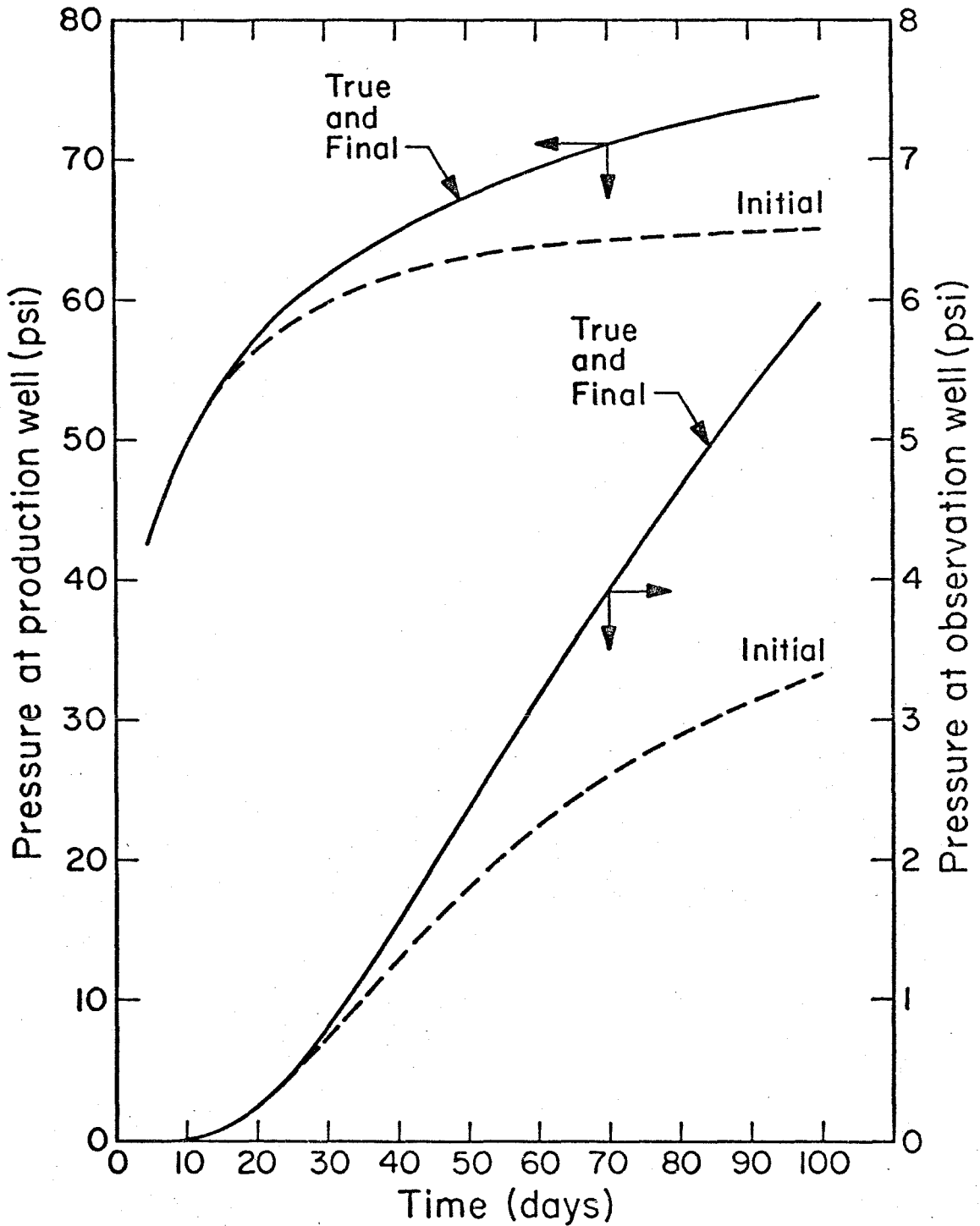


Figure IV-7. Actual and Estimated Pressures at Production and Observation Wells

- True
- - - Initial Guess
- ┌──┐ 5100 ft
- ⊖ Injection Well
- Observation Well

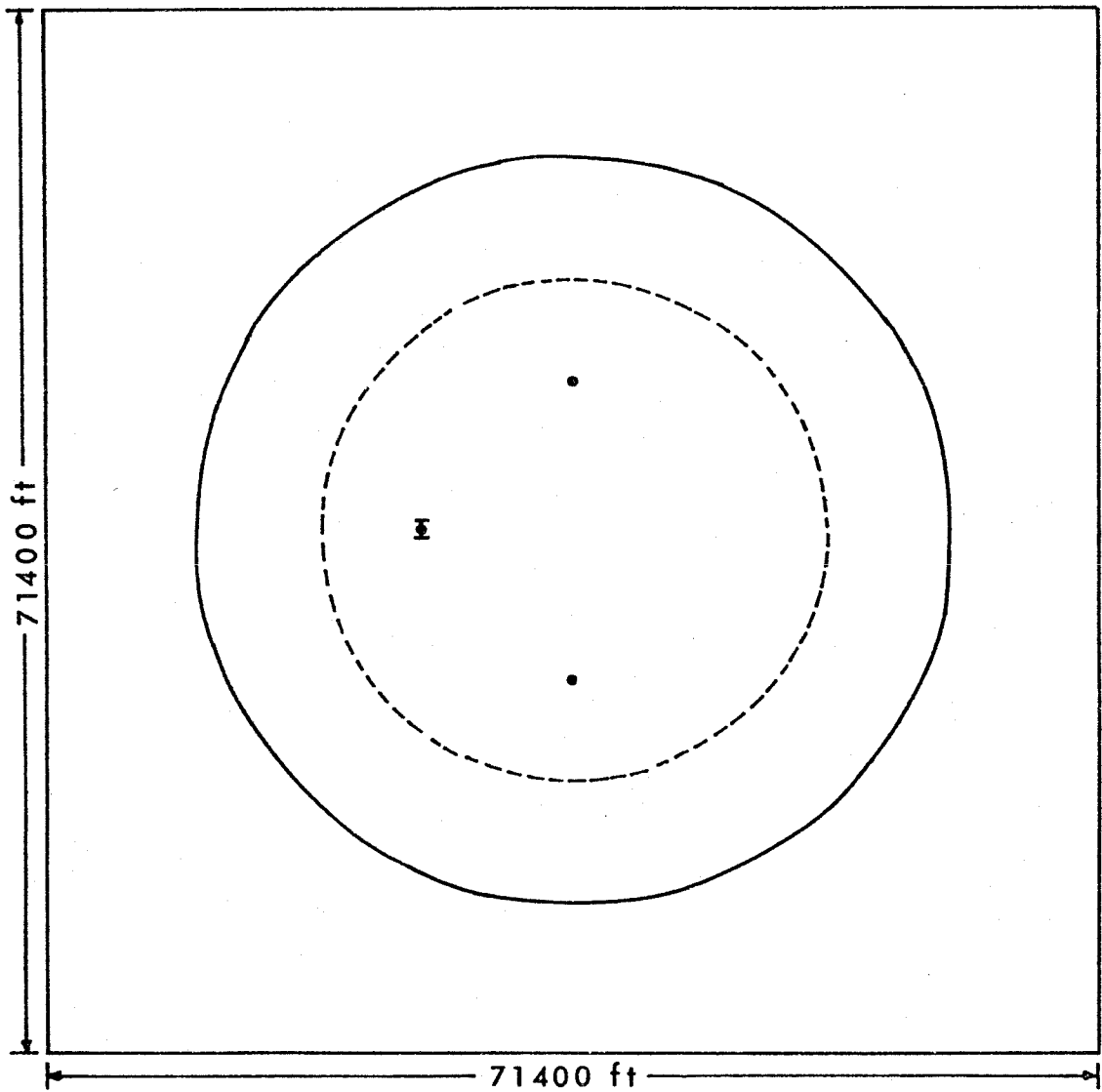


Figure IV-8. Actual and Initial Guess Shape of Reservoir

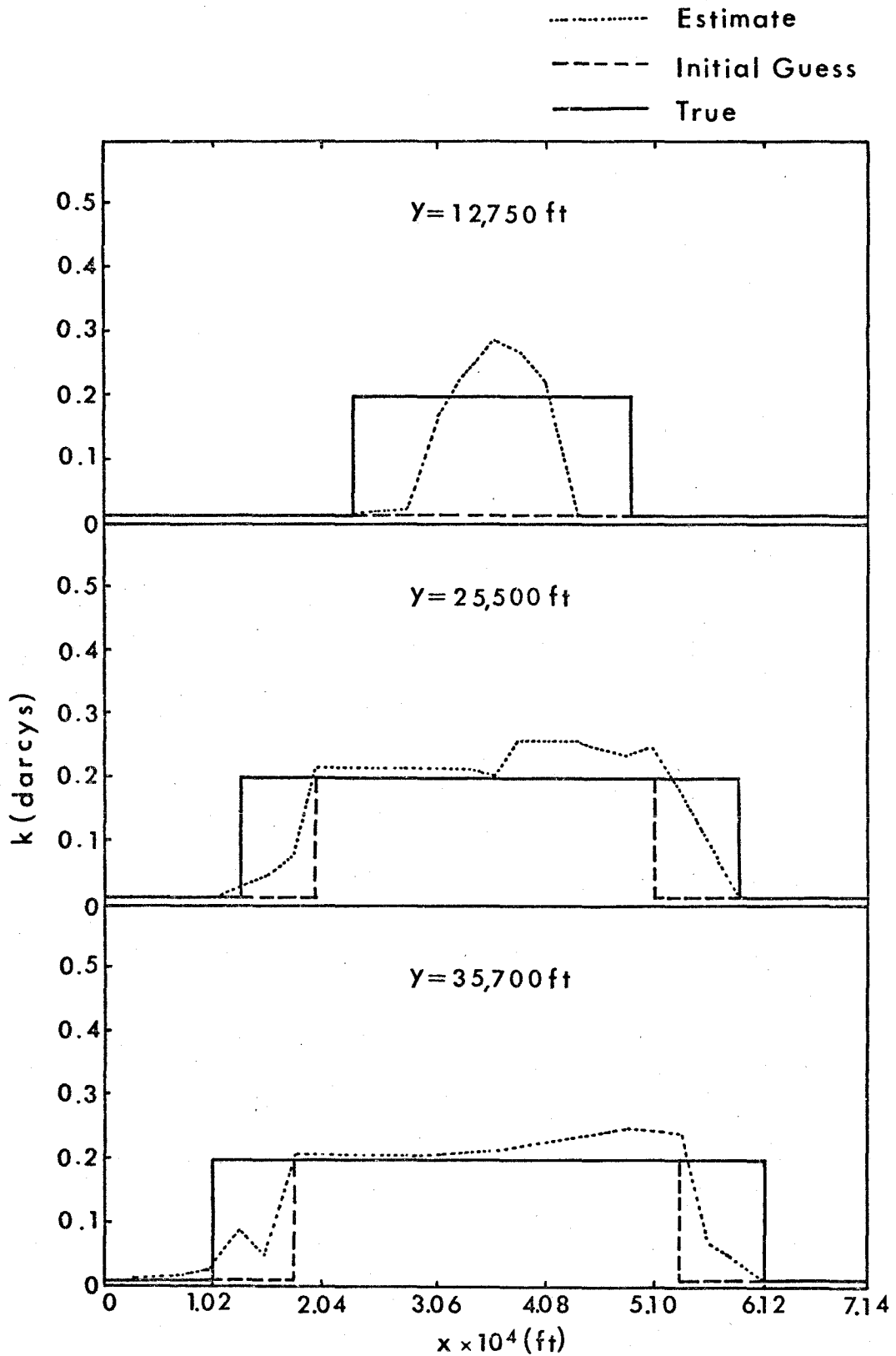


Figure IV-9. Permeability Distributions as Function of x at $y = 12,750$ ft, $25,500$ ft, and $35,700$ ft.

Chapter V

CONCLUSIONS AND REMARKS

In this dissertation nonsequential techniques have been developed for two important classes of parameter estimation problems in distributed parameter systems: (1) constant parameters and (2) spatially varying parameters.

The steepest descent, Gauss-Newton, quasilinearization, and collocation methods, and the optimal control technique are derived for the estimation of constant parameters in partial differential equations and associated boundary conditions. To complete the estimation problem, a method for analyzing the accuracy of constant parameters estimated in partial differential equations is presented. A computational algorithm based on this analysis in conjunction with nonlinear programming is proposed to determine the optimal locations for a fixed number of measurements such that the best estimates can be achieved. It was pointed out that the algorithm proposed actually encompasses the general problem of the optimal location of measurements both in space and time and the problem of the optimal inputs for constant parameter estimation in partial differential equations. The performance of these nonsequential techniques were demonstrated computationally on three examples in the estimation of the conductivity in the heat equation, the activation energy for a single reaction, and the permeabilities in a two-region petroleum reservoir model. It was shown numerically that the parameters can be determined by using the observations measured at the

optimal locations more accurately than utilizing similar measurements made at other points.

Two approaches for estimating spatially varying parameters in partial differential equations have been presented. The first deals with the parameter as a control variable. Then a steepest descent method is derived based on the optimal control theory. The key feature of this method is that the parameter being estimated is treated as a continuous function of position rather than as one assuming discrete values in a number of zones. Although the method was developed for spatially varying parameters, the results may readily be extended to determine time-varying or spatially and time-varying parameters. The second approach considers the parameter as an additional state variable, and then state estimation or filtering techniques can be used. The method of steepest descent appears to be computationally more efficient than filtering because fewer equations must be solved in steepest descent. Both algorithms were employed to estimate the diffusivity in the heat equation. Also, the steepest descent was applied to estimate the permeability distribution in a two-dimensional one-phase petroleum reservoir. Future work is necessary in the development of a method to determine confidence intervals for spatially varying parameter estimates. Estimation of parameters in two-phase reservoir models as proposed in Appendix III-C is also an interesting problem to work on in the future.

The estimation of the location of the boundary (or, equivalently, the shape of a region) has been considered for systems governed by parabolic partial differential equations. A method based on the variation of a functional defined on a variable region is derived. The

feasibility of this method was justified by estimating the locations of the boundaries of a one-dimensional and a two-dimensional petroleum reservoir. It was shown that the method is capable of determining the location of the boundary using the data in the late transient period. Finally, we note that we have considered here only cases of single phase flow, that is, a single partial differential equation for pressure. Subsequent work will be necessary to extend these results to multiphase situations.

REFERENCES

1. A. S. Anderssen and E. T. White, "Parameter estimation by the transfer function method," Chem. Eng. Sci., Vol. 25, 1015-1021 (1970).
2. E. Angel, "Inverse boundary-value problems: elliptic equations," J. Math. Anal. Appl., Vol. 30, 86-98 (1970).
3. M. Aoki and R. M. Staley, "On input signal synthesis in parameter identification," Automatica, Vol. 6, 431-440 (1970).
4. P. C. Badavas and G. N. Saridis, "Response identification of distributed systems with noisy measurements at finite points," Inform. Sci., Vol. 2, 19-34 (1970).
5. Y. Bard, "Comparison of gradient methods for the solution of nonlinear parameter estimation problems," SIAM J. Numer. Anal., Vol. 7, 157-186 (1970).
6. J. V. Beck, "Calculation of thermal diffusivity from temperature measurements," J. Heat Transfer, Trans. ASME, Vol. 85, 181-182 (1963).
7. J. V. Beck, "Transient determination of thermal properties", Nuclear Eng. Design, Vol. 3, 373-381 (1966).
8. J. V. Beck, "Analytical determination of optimum, transient experiments for measurement of thermal properties", Proc. Third Int. Heat Transfer Conference, Vol. 4, 74-80 (1966).
9. J. V. Beck, "Determination of optimum, transient experiments for thermal contact conductance", Int. J. Heat Mass Transfer, Vol. 12, 621-633 (1969).
10. J. V. Beck, "Sensitivity coefficients utilized in nonlinear estimation with small parameters in a heat transfer problem", J. of Basic Eng., Trans. ASME, Vol. 92, 215-222 (1970).

11. J. V. Beck, "Nonlinear estimation applied to the nonlinear inverse heat conduction problem", Int. J. Heat Mass Transfer, Vol. 13, 703-716 (1970).
12. R. Bellman, D. Detchmندی, H. Kagiwada, and R. Kalaba, "On the identification of systems and the unscrambling of data III: one-dimensional wave and diffusion processes", J. Math. Anal. Appl., Vol. 23, 1973-182 (1968).
13. R. Bellman, J. Jacquez, R. Kalaba, and S. Schwimmer, "Quasilinearization and the estimation of chemical rate constants from raw kinetic data", Math. Biosci., Vol. 1, 71-76 (1967).
14. R. Bellman, H. Kagiwada, and R. Kalaba, "Quasilinearization, boundary-value problems and linear programming," IEEE Trans. Automatic Control, Vol. AC-12, 199 (1965).
15. R. Bellman and R. Kalaba, Quasilinearization and Nonlinear Boundary Value Problems, New York: American Elsevier, 1965.
16. G. E. P. Box and H. L. Lucas, "Design of experiments in nonlinear situations", Biometrika, Vol. 46, 77-90 (1959).
17. A. E. Bryson and Y. C. Ho, Applied Optimal Control, Massachusetts: Blaisdell Publishing Company, 1969.
18. O. R. Burggraf, "An exact solution of the inverse problem in heat conduction theory and applications", J. Heat Transfer, Trans. ASME, Vol. 86, 373-382 (1964).
19. J. R. Cannon, "Determination of unknown coefficient in a parabolic differential equation", Duke Math. J., Vol. 30, 313-323 (1963).
20. J. R. Cannon, "Determination of certain parameters in heat conduction problems", J. Math. Anal. Appl., Vol. 8, 188-201 (1964).
21. J. R. Cannon, "Determination of the unknown coefficient $\kappa(u)$ in the equation $\nabla \cdot \kappa(u) \nabla u = 0$ from overspecified boundary data", J. Math. Anal. Appl., Vol. 18, 112-114 (1967).

22. J. R. Cannon, "Determination of an unknown heat source from overspecified boundary data", SIAM J. Numer. Anal., Vol. 5, 275-286 (1968).
23. J. R. Cannon, J. Douglas, and B. F. Jones, "Determination of the diffusivity of an isotropic medium", Int. J. Eng. Sci., Vol. 1, 453-455 (1963).
24. J. R. Cannon and B. F. Jones, "Determination of the diffusivity of an anisotropic medium", Int. J. Eng. Sci., Vol. 1, 457-460 (1963).
25. J. R. Cannon and R. E. Klein, Proc. Joint Automatic Control Conference, Atlanta, Georgia, 1970.
26. W. T. Carpenter, M. J. Wozny, and R. E. Goodson, "Distributed parameter identification using the method of characteristics", J. of Dynamic Systems, Measurement and Control, Trans. ASME, Vol. 93, 73-78 (1971).
27. H. Chernoff, "Locally optimal designs for estimating parameters", Ann. Math. Statist., Vol. 24, 586-602 (1953).
28. W. C. Clements, "A note on determination of the parameters of the longitudinal dispersion model from experimental data", Chem. Eng. Sci., Vol. 24, 957-963 (1969).
29. P. L. Collins and H. C. Khatri, "Identification of distributed parameter systems using finite differences", J. of Basic Eng., Trans. ASME, Vol. 91, 239-245 (1969).
30. R. Collins, Flow of Fluids through Porous Materials, New York: Reinhold Publishing Corporation, 1961.
31. R. Courant and D. Hilbert, Methods of Mathematical Physics, Vol. 1, New York: Interscience Publishers, Inc., 1966.
32. J. E. Crider and A. S. Foss, "An analytic solution for the dynamics of a packed adiabatic chemical reactor", A.I.Ch.E. J., Vol. 14, 77-84 (1968).

33. J. B. Crockett and H. Chernoff, "Gradient methods of maximization", Pacific J. Math., Vol. 5, 33-50 (1955).
34. R. Deutsch, Estimation Theory, New Jersey: Prentice-Hall, Inc., 1965.
35. F. W. Fairman and D. W. C. Shen, "Parameter identification for a class of distributed systems", Int. J. Control, Vol. 11, 929-940 (1970).
36. N. B. Ferguson and B. A. Finlayson, "Transient chemical reaction analysis by orthogonal collocation", Chem. Eng. J., Vol. 1, 327-336 (1970).
37. B. A. Finlayson and L. E. Scriven, "The method of weighted residuals and its relation to certain variational principles for the analysis of transport processes", Chem. Eng. Sci., Vol. 20, 395-404 (1965).
38. B. A. Finlayson and L. E. Scriven, "The method of weighted residuals--a review", Appl. Mech. Rev., Vol. 19, 735-748 (1966).
39. B. A. Finlayson and L. E. Scriven, "On the search for variational principles", Int. J. Heat Mass Transfer, Vol. 10, 799-821 (1967).
40. G. R. Gavalas and J. H. Seinfeld, "Reservoirs with spatially varying properties: estimation of volume from late transient pressure data", Soc. Petrol. Eng. J., in press.
41. I. M. Gelfand and S. V. Fomin, Calculus of Variations, New Jersey: Prentice-Hall, Inc., 1963.
42. R. J. Graham and F. D. Stevenson, "Effects of experimental error on parameter estimation and convergence of a sequential experimental design", Ind. Eng. Chem. Process Des. Develop., Vol. 11, 160-169 (1972).
43. A. H. Haddad and J. B. Cruz, "Observability of constant states of linear systems", Int. J. Control, Vol. 14, 399-400 (1971).

44. Y. Hari, "Optimum boundaries for elliptic systems", J. of Dynamic Systems, Measurement, and Control, Trans. ASME, Vol. 94, 159-164 (1972).
45. M. Hwang and J. H. Seinfeld, "Observability of nonlinear systems", J. Optimiz. Theory Appl., Vol. 10, 67-77 (1972).
46. M. Hwang, J. H. Seinfeld, and G. R. Gavalas, "Optimal least square filtering and interpolation in distributed parameter systems", J. Math. Anal. Appl., Vol. 39, 49-74 (1972).
47. M. Jamshidi, "Application of a parameter-imbedded Riccati equation", IEEE Trans. Auto. Control, Vol. AC-15, 682-683 (1970).
48. B. F. Jones, "The determination of a coefficient in a parabolic differential equation", J. Math. Mech., Vol. 11, 907-926 (1962).
49. J. A. Juusola, D. W. Bacon, and J. Downie, "Sequential statistical design strategy in an experimental kinetic study", Can. J. Chem. Eng., Vol. 47, 796-801 (1972).
50. R. E. Kalaba and K. Spingarn, "Optimal inputs and sensitivities for parameter estimation", J. Optimiz. Theory Appl., Vol. 11, 56-67 (1973).
51. M. G. Kendall and A. Stuart, The Advanced Theory of Statistics, Vol. 2, New York: Hafner Publishing Company, 1961.
52. J. R. Kittrell, W. G. Hunter, and C. C. Watson, "Obtaining precise parameter estimates for nonlinear catalytic rate models", A.I.Ch.E. J., Vol. 12, 5-10 (1966).
53. E. S. Lee, Quasilinearization and Invariant Imbedding, New York: Academic Press, 1968.
54. J. M. Loeb and G. M. Cahen, "More about process identification", IEEE Trans. Aut. Control, Vol. AC-10, 359-361 (1965).
55. D. L. Luckinbill and S. B. Childs, Inverse Problems in Partial Differential Equations, Project Themis, Information Processing Systems, University of Houston, 1968.

56. S. N. Malpani and J. K. Donnelly, "Identification of one-phase flow processes", Can. J. Chem. Eng., Vol. 50, 791-806 (1972).
57. D. W. Marquardt, "An algorithm for least squares estimation of nonlinear parameters", SIAM J. Numer. Anal., Vol. 11, 431-441 (1963).
58. C. S. Matthews and D. G. Russell, Pressure Buildup and Flow Tests in Wells, Monograph Series, Society of Petroleum Engineering, 1967.
59. J. Matyas, "Random optimization", Automation and Remote Control, Vol. 26, 244-251 (1965).
60. R. K. Mehra, "Optimal inputs for linear system identification", Proc. Joint Automatic Control Conference, Stanford, California, 1972.
61. A. Miele, Theory of Optimum Aerodynamic Shapes, New York: Academic Press, 1965.
62. N. E. Nahi and D. E. Wallis, "Optimal inputs for parameter estimation in dynamic systems with white observation noise", Proc. Joint Automatic Control Conference, Boulder, Colorado, 1969.
63. F. J. Perdreauxville and R. E. Goodson, "Identification of systems described by partial differential equations", J. of Basic Eng. Trans. ASME, Vol. 88, 463-468 (1966).
64. M. P. Polis, R. E. Goodson, and M. J. Wozny, "On parameter identification for distributed systems using Galerkin's criterion", Automatica, Vol. 9, 53-64 (1973).
65. J. B. Rosen, "The gradient projection method for nonlinear programming. Part 1. Linear constraints", J. Soc. Indust. Appl. Math., Vol. 8, 181-217 (1960).
66. H. H. Rosenbrock and C. Storey, Computational Techniques for Chemical Engineers, New York: Pergamon Press, 1966.
67. V. E. Sater and F. D. Stevenson, "Use of statistical experimental design in a kinetics study", Ind. Eng. Chem. Process Des. Develop., Vol. 11, 355-359 (1972).

68. J. H. Seinfeld and G. R. Gavalas, "Analysis of kinetic parameters from batch and integral reaction experiments", A.I.Ch.E. J., Vol. 16, 644-647 (1970).
69. J. H. Seinfeld, G. R. Gavalas, and M. Hwang, "Nonlinear filtering in distributed parameter systems", J. of Dynamic Systems, Measurement and Control, Trans. ASME, Vol. 93, 157-163 (1971).
70. J. H. Seinfeld and W. H. Chen, "Estimation of parameters in partial differential equations from noisy experimental data", Chem. Eng. Sci., Vol. 26, 753-766 (1971).
71. M. Shinbrot, "On the analysis of linear and nonlinear dynamic systems from transient-response data", NACA Technical Notes, TN3288, 1954.
72. F. E. Thau, "On optimal filtering for a class of linear distributed parameter systems", J. of Basic Eng., Trans. ASME, Vol. 91, 173-178 (1969).
73. E. Tse, "Information matrix and local identifiability of parameters", Proc. Joint Automatic Control Conference, Columbus, Ohio, 1973.
74. S. G. Tzafestas, "Identification of stochastic distributed parameter systems", Int. J. Control, Vol. 11, 619-624 (1970).
75. J. V. Villadsen and W. E. Stewart, "Solution of boundary-value problems by orthogonal collocation", Chem. Eng. Sci., Vol. 22, 1483-1501 (1967).
76. J. A. Williams, R. J. Adler, and W. J. Zolner, "Parameter estimation of unsteady-state distributed models in the Laplace domain", Ind. Eng. Chem. Fund., Vol. 9, 193-197 (1970).
77. T. K. Yu and J. H. Seinfeld, "Observability and optimal measurement location in linear distributed parameter systems", Int. J. Control, in press.
78. J. L. Lions, Optimal Control of Systems Governed by Partial Differential Equations, New York: Springer-Verlag, 1971.