200
11-15
ANL-7967

7346
ANL-7967

PARAMETER IDENTIFICATION IN NUCLEAR REACTOR SYSTEMS

William Stanley Roman

U of C-AUA-USAEC

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

Prepared for the U.S. ATOMIC ENERGY COMMISSION
under Contract W-31-109-Eng-38

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

The facilities of Argonne National Laboratory are owned by the United States Government. Under the terms of a contract (W-31-109-Eng-38) between the U. S. Atomic Energy Commission, Argonne Universities Association and The University of Chicago, the University employs the staff and operates the Laboratory in accordance with policies and programs formulated, approved and reviewed by the Association.

MEMBERS OF ARGONNE UNIVERSITIES ASSOCIATION

The University of Arizona	Kansas State University	The Ohio State University
Carnegie-Mellon University	The University of Kansas	Ohio University
Case Western Reserve University	Loyola University	The Pennsylvania State University
The University of Chicago	Marquette University	Purdue University
University of Cincinnati	Michigan State University	Saint Louis University
Illinois Institute of Technology	The University of Michigan	Southern Illinois University
University of Illinois	University of Minnesota	The University of Texas at Austin
Indiana University	University of Missouri	Washington University
Iowa State University	Northwestern University	Wayne State University
The University of Iowa	University of Notre Dame	The University of Wisconsin

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights.

Printed in the United States of America
Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151
Price: Printed Copy \$3.00; Microfiche \$0.95

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

PARAMETER IDENTIFICATION IN
NUCLEAR REACTOR SYSTEMS

by

William Stanley Roman
Reactor Analysis and Safety Division

Based on a dissertation submitted to
the School of Engineering and Applied Science
University of Virginia
in partial fulfillment of the requirements
for the degree of
Doctor of Philosophy
in the field of Nuclear Engineering

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

September 1972

100-100000

TABLE OF CONTENTS

	<u>PAGE</u>
ABSTRACT.....	7
I. INTRODUCTION.....	8
A. Background.....	9
B. Lumped-parameter Identification.....	11
C. Lumped-parameter Identification in Nuclear Systems.....	11
D. Distributive-parameter Identification.....	11
E. Objective and Organization of Dissertation.....	12
II. QUASI-LINEARIZATION AND LUMPED-PARAMETER IDENTIFICATION.....	14
A. Historical Background.....	14
B. Second-order Differential Equation.....	14
C. Systems of Equations.....	16
D. Superposition and Computer Storage.....	19
E. Lumped-parameter Identification.....	19
F. Advantages and Disadvantages of Quasi-linearization.....	21
III. PARAMETER IDENTIFICATION IN A NUCLEAR REACTOR SYSTEM.....	22
A. LMFBR Model.....	22
B. One-neutron-energy-group Model.....	22
C. Determination of Criticality Conditions.....	25
D. Identification of Two Temperature- feedback Coefficients.....	27
1. Effect of Number and Accuracy of Measurements on Identification.....	30
2. Effect of Magnitude of Parameters and Criterion Function on Identification.....	32
E. Identification of Four Temperature- feedback Coefficients.....	33
F. Two-neutron-energy-group Model.....	34
G. Discussion of Results and Conclusions.....	39
IV. DISTRIBUTIVE-PARAMETER IDENTIFICATION.....	41
A. Introduction.....	41
B. Distributive-parameter Model and Criterion Function.....	42
C. Parameter Identification and Gradient Techniques.....	43
D. Gradient Search Directions.....	44

TABLE OF CONTENTS (Contd.)

	<u>PAGE</u>
E. Gradient Evaluation.....	48
F. Selection of ρ_1	49
G. Convergence Criterion.....	51
H. Summary and Algorithm for Distributive-parameter Identification.....	52
V. NUMERICAL RESULTS OF DISTRIBUTIVE PARAMETER IDENTIFICATION.....	54
A. Introduction.....	54
B. Parabolic Partial Differential Equation.....	55
1. Identification of One Parameter.....	57
2. Identification of Two Parameters.....	58
3. Identification of Three Parameters.....	59
C. Hyperbolic Partial Differential Equations.....	61
D. Space-Time-dependent Nuclear Reactor Model.....	64
E. Discussion of Results.....	68
VI. CONCLUSIONS AND RECOMMENDATIONS.....	70
APPENDICES.....	71
A. Development of Feedback and Thermal- hydraulic Model.....	71
B. Development of Newton and Gauss-Newton Gradient Techniques.....	80
C. Method of Conjugate Directions.....	84
ACKNOWLEDGMENTS.....	88
REFERENCES.....	89

LIST OF TABLES

<u>TABLE</u>	<u>TITLE</u>	<u>PAGE</u>
I	One-neutron-energy-group Coefficients.....	25
II	κ Values at End of Each Iterative Cycle.....	27
III	Effect of Measurement Error on the Accuracy Identification.....	31
IV	Accuracy of Identification Based on the Magnitude of the Feedback Coefficients.....	32
V	Effect of Equal Values of W_1 and W_2 on the Accuracy of the Parameter Identification.....	33
VI	Identification of Four Temperature Coefficients.....	34
VII	Two-neutron-energy-group Coefficients.....	38
VIII	Identification of Temperature Coefficients in Two-neutron-energy-group Model.....	39
IX	Gradient Search Direction.....	53
X	Identification of Two Parameters in a Parabolic Equation.....	59
XI	Identification of Three Parameters in a Parabolic Equation.....	60
XII	Effect of μ^* Value on Conjugate- Gradient Technique.....	60
XIII	Parameter Identification Based Upon $u(L,t)$ Measurements.....	63
XIV	Parameter Identification Based Upon $v(0,t)$ Measurements.....	63
XV	Parameter Identification Based Upon $u(L,t)$ and $v(0,t)$ Measurements.....	63
XVI	Identification of Parameters for Nonlinear Nuclear Reactor Model.....	67
XVII	Parameter Identification for Spatially Dependent Reactor Transients.....	68
A.I	Thermohydraulic Parameters.....	78

LIST OF FIGURES

<u>FIGURE</u>	<u>TITLE</u>	<u>PAGE</u>
1	Comparison of Control and Identification Problems.....	9
2	Flow Chart for Criticality Problem.....	28
3	Comparison of Feedback and No-feedback Models for One Neutron-energy Group.....	29
A.1	Top View of Unit-cell Configuration.....	71
A.2	Longitudinal View of Unit-cell Configuration.....	72

PARAMETER IDENTIFICATION IN NUCLEAR REACTOR SYSTEMS

by

William Stanley Roman

ABSTRACT

Several techniques are developed for the identification of unknown parameters in lumped and distributive parameter models of nuclear reactor systems. Specifically, a set of algorithms are developed for updating initial parameter estimates by minimizing a least squares criterion function using simulated measurements of the system variables.

For the space-dependent-only lumped parameter system, the quasi-linearization technique is shown to be an effective method of identifying parameters in a nonlinear model of a liquid metal fast breeder reactor (LMFBR). In addition to demonstrating the applicability of the quasi-linearization technique to nuclear reactor models, studies were made to illustrate the effect of initial parameter estimates, measurement errors, and number of measurements upon the accuracy of the identification.

To identify parameters in a distributive-parameter system, a set of quasi-Newton gradient techniques are shown to be effective methods for parameter identification. The gradient techniques that were analyzed are the Gauss-Newton, conjugate gradient, and variable metric. Results of the analysis showed that the Gauss-Newton technique was superior to the other methods in both accuracy and efficiency. These results were obtained for a time dependent extension of the nonlinear LMFBR model analyzed for the lumped-parameter system, and two linear models of heat transfer and fluid flow processes that are encountered in the analysis of nuclear reactor systems.

I. INTRODUCTION

A. Background

The role of the engineer has always been to predict the performance of a physical system by means of a mathematical model. In developing a mathematical model, the engineer must often use inexact or incomplete knowledge of the system to reconcile physical theory and experimental measurements. It is this problem of perfecting the model to describe a physical system that the theory of identification seeks to remedy.

In general, the identification process can be separated into two categories based on the initial knowledge of the system. If the nature of the system is totally unknown, then the engineer is faced with the so-called "black box" problem where only the system inputs and outputs are known. However, physical theory frequently provides the mathematical equations that approximately describe the nature of the system, but some of the specific values of the parameters are unknown. It should be evident that most engineering problems are of this type. Generally, the unknown parameters are the coefficients of the dependent variables in the mathematical model. The coefficients can be constants, but they can also be functions of the independent and dependent variables. But it is possible to write these variable-dependent coefficients as a function of unknown constants and known mathematical functions, e.g., a power series or a Fourier series expansion. Thus, all the unknown parameters to be identified can be considered as constants.

In general, the unknown parameters are not directly measureable and a technique must be developed to find these parameters in terms of the measureable quantities of the system. To develop such a technique, it is necessary to provide three basic elements:

1. Plant Model;
2. Criterion Function;
3. Parameter Modification.

In plant modeling, the systems can be described as lumped-parameter models, i.e., those described by ordinary differential equations, or distributed-parameter models, i.e., those described by partial differential equations. This study will be concerned with both models. With respect to the lumped-parameter case, however, the system to be examined is based on a steady-state spatial model of a nuclear reactor core as opposed to the usual time-dependent parameter model, e.g., the point kinetics equations. A well-developed time-dependent model technique will be employed to analyze this spatially dependent model.

The criterion function is often called the performance index or cost function in the control literature, and it yields a measure of the accuracy of the plant model with respect to the physical plant. It provides the technique for reducing the plant measurements to a useful form and thus provides with the plant equations the mathematical basis for the parameter

identification. In this study, the least-squares error criterion will be employed exclusively as the criterion function. It is a positive-definite functional based on the square of the difference between the observed or actual system measurements and the calculated results of the plant model.

Parameter modification is the technique developed to upgrade the initial estimate of the unknown parameters based on the information supplied by the plant equations and the criterion function. The specific algorithm chosen may be independent of the form of the plant-model criterion function or it may be an integral part of either one or both of these elements of the identification scheme.

The identification problem has been closely associated with the optimal control problem, and many of the techniques used to solve the control problem can be employed for the identification problem. In the control problem, the plant is known and the input is determined to obtain the desired output; the identification problem is concerned with determining the plant when the input and output are known. This difference is illustrated in Fig. 1. A more complete breakdown of the control and identification problems for lumped-parameter systems is presented by Lee.¹

Fig. 1.
Comparison of Control and Identification Problems.

B. Lumped-parameter Identification

In surveying the literature of lumped-parameter identification techniques, one is faced with a multitude of methods that make a complete survey impossible. Thus, the survey will be limited to the more prominent techniques now being used. A recent survey by Cuenod and Sage² presents some of the methods employed in process control and compares their performance for a simple problem.

The original techniques employed for plant identification were restricted to linear systems and based on the transfer-function analysis. Using a sinusoidal input to the system, an experimental Bode diagram is constructed and then an analytical expression is obtained for the transfer function. This technique is presented in many texts on automatic control and is clearly described by D'Azzo and Houpis.³ The Bode-diagram analysis is made in the frequency domain; a similar analysis can be made in the time domain using the convolution integral relating the input and output of the system. The convolution integral is evaluated at discrete time intervals, and a set of equations for the plant model is obtained. This process is called numerical deconvolution⁴ in the literature. If noise is present in the plant

measurements, correlation techniques⁵ are employed to obtain information about the plant. Fourier-transform techniques have been used to obtain a spectral density function for the system, and recently the computational technique of the fast Fourier transform⁶ has increased the use of this method.

Previously mentioned techniques do not make use of the criterion function to obtain the solution. The next class of methods described are based on optimizing the criterion function. These techniques originated in the optimization of explicit functions of an algebraic form, and an excellent review of these minimization techniques exists.⁷ These methods are usually referred to as search techniques and make use of the criterion function at several points to obtain the minimum value. If only one parameter is unknown, many very efficient techniques exist.⁷⁻⁹ When the number of unknown parameters is small, it is possible to eliminate each unknown parameter sequentially while the remaining parameters are held constant. This process continues until a minimum is obtained for all the unknown parameters. As the number of unknown parameters increases, this technique converges very slowly, and a method of varying all the unknown parameters simultaneously is used. Initially the parameters are varied randomly until a search direction is found that will minimize the criterion function. This process is repeated until the criterion function satisfies some convergence criterion. These search techniques are outlined by Wilde and Beightler.⁹

Search techniques that use the slope of the criterion function as the parameters are varied are known as gradient techniques. These procedures have been applied to the control problem extensively. Probably the best known and used gradient technique is the steepest-descent method,¹⁰ in which the search direction for the unknown parameters is along a line parallel to the local gradient of the criterion function with respect to the unknown parameters. However, the steepest-descent technique becomes a very slow process as the minimum of the criterion function is approached. To increase the convergence rate, the criterion function is approximated by the first three terms of a Taylor Series expansion to yield a quadratically convergent method. This technique, called Newton's method, is outlined by Fletcher¹¹ and Powell.¹² Newton's method has the drawback of requiring the computation of the second partial derivatives, which can lead to considerable numerical work. Several modifications of Newton's method, called quasi-Newton, avoid the computation of second partial derivatives. A comparison of gradient methods by Bard¹³ for lumped-parameter models indicated that quasi-Newton methods yielded excellent results for specific classes of problems.

A class of methods have been developed for stochastic systems based on filtering theory. In this class of techniques the term estimation is often used to describe the identification process. The basis for these methods is the Wiener filter as developed in Davenport and Root¹⁴ and Lee.¹ Originally, the technique was based on a frequency domain analysis, but Kalman¹⁵ derived a similar result for the time domain. These results form the basis for many estimation procedures developed during the past decade. One of the most recent developments has been stochastic approximation,¹⁶ which can be thought of as an extension of the gradient method for a stochastic system. These techniques will not be used for this analysis since the assumption of little or no noise in the plant model will be made.

The last class of identification techniques to be outlined are those which had their origin in the solution of the optimal control problem by dynamic programming.¹⁷ Originally, these methods were employed to transform nonlinear, two-point boundary-value problems into a sequence of linear differential equations. Quasi-linearization¹⁸ and invariant imbedding¹⁹ are the two most prominent of these techniques. Quasi-linearization will be the technique used to solve the spatially dependent lumped-reactor-core identification problem, and its development will be given in Ch. II. The invariant imbedding approach generates a sequential relationship by imbedding the original two-point boundary-value equations into a class of single-point boundary-value problems. A comparison of these techniques and their interconnections for variational problems are given by Bellman and Kalaba.²⁰ Comparison between quasi-linearization and gradient techniques for two-point boundary-value problems are given by Kenneth and McGill.²¹ Further references for problems that have been solved by quasi-linearization and invariant imbedding are found in Bellman and Kalaba¹⁸ and Lee.¹⁹

C. Lumped-parameter Identification in Nuclear Systems

Although these techniques have been used extensively to solve the optimal control problem in nuclear systems, their use for parameter identification has been limited to the point kinetics model for reactors. An extensive review of the optimal control of nuclear systems has been given by Lipinski.²²

Sage and Ellis²³ developed a sequential technique based on invariant imbedding to solve the point kinetics model for reactor startup and a nuclear rocket model. Sage and Masters²⁴ extended this method to nonlinear discrete systems and also used a nonlinear point kinetics model. Habegger²⁵ used the Kalman filter technique to identify parameters in reactor systems. Use of quasi-linearization to determine the delayed-neutron lifetime, and ramp rates in the point kinetics model, has been made.²⁶ The basis for the spatial identification method for reactor models were the results of Habegger and Hsu's²⁷ solution of the two-point nonlinear boundary-value problems.

D. Distributed-parameter Identification

The techniques for distributed-parameter identification have been limited as compared with the lumped-parameter methods. Many of the techniques for distributed-parameter systems are based on the solution of the optimal control problem for these models.^{28,29} Initially, the conductivity constant in a one-dimensional heat-diffusion equation was identified by Jones³⁰ and by Jones and Douglas.³¹ Their technique was based on a linear equation and the use of a spatial averaging technique to eliminate first the spatially dependent variable to obtain a time-dependent equation to be solved by discretizing the variables in the time domain. Perdreauxville and Goodson³² employed a weighted spatial-averaging technique and then used polynomial approximations to obtain a set of algebraic equations in terms of the unknown coefficients. However, their approach is limited to systems for which a weighting function can be developed.

Saridis and Badavas³³ applied a stochastic approximation scheme to a linear system, which required the use of orthonormal piecewise-continuous functions to approximate the system. The identification was then made for the coefficients for this set of functions. The "state identification problem" was solved by Phillipson and Mitter³⁴ in which the initial conditions and original boundary conditions are determined by measurements of the system variables. Their technique is applicable to linear parabolic and hyperbolic equations, and uses Galerkin's method to approximate the system variables.

Quasi-linearization procedures were used by Croce-Spinelli³⁵ for a nonlinear ordinary differential equation after the original partial differential equation had been discretized in the time domain. Results of this analysis were inaccurate for nonlinear problems, since the measurements of the system variable were made only at the spatial boundary at various time intervals. A simplified method of obtaining parameters using finite differences was developed by Collins and Khatri.³⁶ Their technique consisted of manipulating the original partial differential equations into a set of known functions and a linear combination of unknown parameters. Then a matrix of measurement values was used to compute the known functions, and the unknown parameters were determined by matrix inversion. However, this matrix can become singular unless care is taken in selecting the measurements. Also, all variables must be written in an explicit form to construct the solution matrix.

Seinfeld³⁷ used the steepest-descent algorithm with a least criterion function to identify parameters in parabolic and hyperbolic systems. The problem that is encountered in this technique is poor convergence, associated with all steepest-descent techniques. Also, no method was employed to optimize parametric changes from iteration to iteration. A modification of the Gauss-Newton technique, which is a quasi-Newton method, was applied to linear parabolic systems by Herbold.³⁸ This technique is based on a least-squares criterion and approximates Newton's method without use of the second derivative function. If the initial estimates for the parameters are poor and the measurements of the system are in error, convergence cannot be guaranteed.

E. Objective and Organization of Dissertation

There are two objectives in this dissertation: first, to develop the quasi-linearization technique as an efficient method of obtaining accurate parameter identification in a spatially dependent lumped-parameter model of a nuclear reactor core; second, to develop a set of quasi-Newton methods to solve the parameter-identification problem for distributed-parameter systems described by parabolic and hyperbolic partial differential equations.

In Ch. II, the quasi-linearization technique is developed for the two-point boundary-value problem and the parameter-identification problem for a spatially dependent lumped-parameter model. Numerical results of this analysis for models with one and two neutron-energy groups of an LMFBR core are presented in Ch. III. In Ch. IV, several quasi-Newton techniques are developed for distributed-parameter models. Also, several methods for one-dimensional search techniques are developed. Three models of distributed-

parameter systems are presented in Ch. V, and the numerical results for the quasi-Newton identification techniques are given. In Ch. VI, the results of the analysis are summarized, and recommendations for further research are given.

II. QUASI-LINEARIZATION AND LUMPED-PARAMETER IDENTIFICATION

A. Historical Background

Parameter identification for a lumped-parameter system can be formulated as a general, nonlinear, multipoint boundary-value problem.¹⁹ The solution of this problem directly identifies the unknown parameters. The quasi-linearization (hereafter referred to as QL) technique is an indirect method for the solution of nonlinear, multipoint boundary-value problems. The QL technique consists of producing a sequence of approximating functions which converge rapidly to the solution of the original nonlinear problem. Thus it differs from the usual indirect procedure of systematically varying arbitrarily chosen initial conditions until the remaining boundary conditions are satisfied.

In many ways, the QL procedure is similar to the Newton-Raphson technique for finding the roots of a nonlinear algebraic equation. In fact, many authors refer to the technique as the Generalized Newton-Raphson method for functional equations. The basic generalization to functional equations was accomplished by Kantorovitch.³⁹ Use of the technique to solve boundary-value problems was first suggested by Hestenes,⁴⁰ who called the method "differential variations." In solving the Riccati equation using dynamic programming, Bellman⁴¹ noted that the modified equation possessed certain properties of linear equations and thus the term "quasi-linearization" was used. Further applications to boundary-value problems were developed by Kalaba,⁴² who presented proofs of the convergence of the procedure for a second-order differential equation with two-point boundary conditions. The proofs of convergence were extended to N-dimensional systems by McGill and Kenneth.⁴³ All of these proofs are based on the existence and uniqueness of the QL operation.

In this chapter, the emphasis will be placed on the computational aspects of the technique rather than on the theoretical derivations of the method. These derivations are presented in the previously mentioned references, and are summarized by Bellman and Kalaba.¹⁸

B. Second-order Differential Equation

In general, lumped-parameter systems can be considered to be modeled by a set of first-order, nonlinear differential equations. However, to illustrate clearly the QL technique, a simple second-order equation is chosen here; the use of the QL technique for an N^{th} -order system will be given in Sect. II.C. Consider the following second-order nonlinear ordinary differential equation over the range $0 \leq x \leq L$:

$$\frac{d^2 u(x)}{dx^2} = F[u(x), x] , \quad (1)$$

with boundary conditions

$$u(0) = b_1; \quad u(L) = b_2. \quad (2)$$

An initial approximation $u_0(x)$ for the function $u(x)$ is made based on the available information describing the behavior of $u(x)$. It is not necessary for this initial approximation to satisfy the boundary conditions. The function $F[u(x), x]$ can now be expanded about $u_0(x)$ by use of a Taylor series expansion that is truncated after the first-order terms:

$$F[u(x), x] = F[u_0(x), x] + \frac{\partial F[u_0(x), x]}{\partial u(x)} [u(x) - u_0(x)]. \quad (3)$$

In combining Eqs. 1 and 3 a linear differential equation with varying coefficients is formed:

$$\frac{d^2 u(x)}{dx^2} = \frac{\partial F[u_0(x), x]}{\partial u(x)} [u(x) - u_0(x)] + F[u_0(x), x]. \quad (4)$$

A recurrence relationship can now be formulated from Eq. 4 for the $(i+1)$ approximation to the original nonlinear equation, Eq. 1; the x dependence of u in $F(u, x)$ has been omitted for clarity:

$$\frac{d^2 u_{i+1}(x)}{dx^2} = \frac{\partial F(u_i, x)}{\partial u} u_{i+1}(x) + F(u_i, x) - \frac{\partial F(u_i, x)}{\partial u} u_i(x). \quad (5)$$

The term $F(u_i, x)$ corresponds to $F[u(x), x]$ evaluated for values of $u_i(x)$ whereas $\partial F(u_i, x)/\partial u$ is $\partial F[u(x), x]/\partial u$ evaluated for $u_i(x)$ values. Although Eq. 5 is linear, it has varying coefficients and, in general, it cannot be solved analytically. However, since it is linear, a standard technique for a numerical solution of linear boundary-value problems can be used.

The iterative process is continued until convergence is obtained by satisfying the following criterion:

$$\begin{array}{c} \text{MAX} \\ 0 \leq x \leq L \end{array} \left| \frac{u_{i+1}(x) - u_i(x)}{u_{i+1}(x)} \right| \leq \mu. \quad (6)$$

Selection of the μ value depends upon the desired accuracy of the final solution. The rate of convergence is the reason that the QL procedure is employed.

The QL operation not only linearizes the original nonlinear equation, but also provides an iterative technique that is quadratically convergent as the solution is approached. Convergence of the linearized equations is dependent on a "good" initial approximation $u_0(x)$. Proofs for the convergence of the QL technique, found in the references previously cited, are

based on sufficiency conditions, and often convergence occurs when these conditions are not satisfied. Often monotone convergence occurs provided that the function $F[u(x), x]$ is strictly concave (convex) near the region of the solution.

C. System Equations

QL procedures are now applied to systems described by a set of N first-order nonlinear differential equations. In vector form they are

$$d\mathbf{u}(x)/dx = \mathbf{F}[\mathbf{u}(x), x], \quad (7)$$

where $\mathbf{u}(x)$ and $\mathbf{F}[\mathbf{u}(x), x]$ are N -dimensional column vector and nonlinear vector functions, respectively. The boundary conditions for this set of equations are given by K conditions at $\mathbf{u}(0)$ and $(N-K)$ conditions at $\mathbf{u}(L)$:

$$\mathbf{A} \mathbf{u}'(0) = \mathbf{b}; \quad \mathbf{C} \mathbf{u}''(L) = \mathbf{d}, \quad (8)$$

where $\mathbf{u}'(0)$ is a K -dimensional vector and $\mathbf{u}''(L)$ is a $(N-K)$ -dimensional vector with $\mathbf{A}$ and $\mathbf{b}$ being a K -dimensional square matrix and column vector, respectively, and $\mathbf{C}$ and $\mathbf{d}$ being a $(N-K)$ -dimensional square matrix and column vector, respectively. If $\mathbf{A}$ and $\mathbf{C}$ are identity matrices, the boundary conditions have the form

$$\mathbf{u}'(0) = \mathbf{b}; \quad \mathbf{u}''(L) = \mathbf{d}. \quad (9)$$

With the boundary conditions given by Eq. 8 or Eq. 9 it is not necessary that each of the variables in $\mathbf{u}(x)$ be given a value at either end point, but that there exist N independent boundary conditions. Thus, some variables may have known values at both boundaries while other variables are unspecified at either boundary.

After a set of initial approximations for the variables $\mathbf{u}(x)$ are chosen, a recurrence relationship can be written for the $(i+1)$ approximation:

$$d\mathbf{u}_{i+1}(x)/dx = \mathbf{F}[\mathbf{u}_i(x), x] + \mathbf{H}(\mathbf{u}_i) \left[\mathbf{u}_{i+1}(x) - \mathbf{u}_i(x) \right], \quad (10)$$

where $\mathbf{H}(\mathbf{u}_i)$ represents the N -dimensional square Jacobian matrix evaluated at $\mathbf{u}_i(x)$:

$$\underline{H}(\underline{u}_1) = \begin{bmatrix} \frac{\partial F_1}{\partial u_1}(\underline{u}_1, x) & \frac{\partial F_1}{\partial u_2}(\underline{u}_1, x) & \cdots & \frac{\partial F_1}{\partial u_N}(\underline{u}_1, x) \\ \frac{\partial F_2}{\partial u_1}(\underline{u}_1, x) & & & \vdots \\ \vdots & & & \vdots \\ \frac{\partial F_N}{\partial u_1}(\underline{u}_1, x) & \cdots & \cdots & \frac{\partial F_N}{\partial u_N}(\underline{u}_1, x) \end{bmatrix} \quad (11)$$

The boundary conditions for Eq. 10 are given by

$$\underline{A} \underline{u}'_{i+1}(0) = \underline{b} ; \quad \underline{C} \underline{u}''_{i+1}(L) = \underline{d} . \quad (12)$$

As mentioned previously, the quasi-linearized equation is linear, but in general cannot be solved analytically because of the variable coefficients. Since Eq. 10 is linear, the principle of superposition is valid, and the total solution of Eq. 10 is formed by a set of particular solutions and (N-K) sets of homogeneous solutions. The (N-K) sets correspond to the number of unknown initial conditions. The total solution can be formed by the following vector equation:

$$\underline{u}_{i+1}(x) = \underline{p}_{i+1}(x) + \underline{\psi}_{i+1}(x) \underline{\alpha}_{i+1} , \quad (13)$$

where $\underline{p}_{i+1}(x)$ is an N-dimensional column vector of the particular solution, $\underline{\psi}_{i+1}(x)$ is an N by (N-K) homogeneous solution matrix, and $\underline{\alpha}_{i+1}$ is an (N-K) column vector of integration constants.

The particular solution vector $\underline{p}_{i+1}(x)$ is obtained by the solution of the following differential equation:

$$d\underline{p}_{i+1}(x)/dx = \underline{F}(\underline{u}_1, x) + \underline{H}(\underline{u}_1) \left[\underline{p}_{i+1}(x) - \underline{u}_1(x) \right] . \quad (14)$$

The homogeneous solution matrix is found by solving the following equation:

$$d\underline{\psi}_{i+1}(x)/dx = \underline{H}(\underline{u}_1) \underline{\psi}_{i+1}(x) . \quad (15)$$

Initial conditions for these equations are selected so that the total solution, Eq. 13, satisfies the boundary conditions given by Eq. 12. To specify the boundary for $\underline{p}_{i+1}(x)$ and $\underline{\psi}_{i+1}(x)$, it is necessary to partition these matrices:

$$\underline{p}_{i+1}(x) = \begin{bmatrix} p'_{i+1}(x) \\ p''_{i+1}(x) \end{bmatrix}; \quad \underline{\psi}_{i+1}(x) = \begin{bmatrix} \psi'_{i+1}(x) \\ \psi''_{i+1}(x) \end{bmatrix}, \quad (16)$$

where $p'_{i+1}(x)$ is a K -dimensional vector, $p''_{i+1}(x)$ is an $(N-K)$ -dimensional vector, $\psi'_{i+1}(x)$ is a K by $(N-K)$ -dimensional matrix, and $\psi''_{i+1}(x)$ is an $(N-K)$ -dimensional square matrix.

The initial conditions for $\underline{p}_{i+1}(x)$ are obtained from Eq. 12:

$$\underline{A} \underline{p}_{i+1}(0) = \underline{b}, \quad (17)$$

and $\underline{\psi}_{i+1}(0)$ must satisfy the conditions

$$\underline{A} \underline{\psi}_{i+1}(0) \underline{\alpha}_{i+1} = \underline{0}. \quad (18)$$

For the remaining $(N-K)$ boundary conditions at $x = 0$ the values for $\underline{\alpha}_{i+1}$ are determined by substituting Eq. 13 for $\underline{u}_{i+1}(L)$ in Eq. 8 to obtain $(N-K)$ algebraic equations

$$\underline{C} \left\{ \underline{p}_{i+1}(L) + \underline{\psi}_{i+1}(L) \underline{\alpha}_{i+1} \right\} = \underline{d}. \quad (19)$$

With the solution for $\underline{\alpha}_{i+1}$, the initial conditions for $\underline{p}_{i+1}(x)$ and $\underline{\psi}_{i+1}(x)$ can now be arbitrarily chosen provided the values satisfy Eqs. 17 and 18. The following choice was made for the initial conditions:

$$\begin{aligned} \underline{A} \underline{p}_{i+1}(0) &= \underline{b}; & \underline{\psi}_{i+1}(0) &= \underline{0}; \\ \underline{p}_{i+1}''(0) &= \underline{0}; & \underline{\psi}_{i+1}''(0) &= \underline{I}, \end{aligned} \quad (20)$$

where $\underline{I}$ is the identity matrix. With this set of initial conditions the missing $(N-K)$ initial conditions for $\underline{u}_{i+1}(x)$ are given by the values of the integration constants $\underline{\alpha}_{i+1}$. The iterative procedure for this technique is as follows:

1. Choose an initial approximation, $\underline{u}_0(x)$, for the system variables.
2. Use the values of $\underline{u}_0(x)$ for $\underline{u}_1(x)$.
3. Evaluate the Jacobian matrix $\underline{H}(\underline{u}_1)$.

4. With initial conditions Eq. 20, solve for $p_{i+1}(x)$ and $\psi_{i+1}(x)$, using Eqs. 14 and 15.
5. Solve for α_{i+1} using Eq. 19.
6. Obtain the total solution $u_{i+1}(x)$ using Eq. 13.
7. Test for convergence using Eq. 6 for all $u_{i+1}(x)$ values; if convergence is not satisfied, repeat steps 3 through 7 using the values of $u_{i+1}(x)$ for $u_i(x)$.

D. Superposition and Computer Storage

Superposition was used to transform the boundary-value problem given by Eq. 13 into an initial-value problem to facilitate numerical computation. An initial-value problem is well suited to digital computation as compared with a boundary-value problem, which requires a more sophisticated numerical algorithm. In using the above algorithm it is necessary to store the solutions of the $p_{i+1}(x)$ vector and the $\psi_{i+1}(x)$ matrix at each of the spatial mesh points in the integration procedure in order to calculate the total solution of $u_{i+1}(x)$ using Eq. 13. For a large-dimensional system of equations or for many spatial mesh points, the storage requirements could easily surpass the computer capacity.

Another technique⁴⁴ can be used when the need to store the values at $p_{i+1}(x)$ and $\psi_{i+1}(x)$ at each mesh point is unnecessary. Since Eq. 19 requires only the values at $p_{i+1}(L)$ and $\psi_{i+1}(L)$ to obtain α_{i+1} , which are the missing initial conditions for $u_{i+1}(x)$ the total solution can be obtained by direct integration of Eq. 10 from 0 to L. Therefore, a trade-off has been made between computer storage and the need to solve an added set of differential equations. Both of these techniques were employed in the examples given in Ch. III, but there was very little difference in computational time due to the limited number of variables. Also, the IBM-360 computer used for this analysis had sufficient storage for both the $p_{i+1}(x)$ and $\psi_{i+1}(x)$ values.

E. Lumped-parameter Identification

The QL procedure will now be extended to identify parameters in models of nonlinear lumped-parameter systems. This technique has been used by Lee¹⁹ to investigate chemical engineering problems and by Larson⁴⁵ for aeronautical modeling. Essentially, the unknown parameters are coupled with the system differential equations and are treated as variables.

Consider the following set of first-order nonlinear ordinary differential equations:

$$du(x)/dx = F[u(x,a),x,a] \quad (21)$$

with the associated boundary conditions given by Eq. 8. The system is N^{th} order, with a being an M -dimensional constant vector of unknown parameters.

These parameters are to be determined from a set of spatial measurements, $\underline{y}(x)$, where

$$\underline{y}(x) = \underline{h}(x, \underline{u}) \quad (22)$$

and where $\underline{h}(x, \underline{u})$ is a transformation that relates the system variables to the measurements of the system. If the system variables are directly measurable, then

$$\underline{h}(x, \underline{u}) = \underline{u}(x) . \quad (23)$$

Also, the assumption will be made that the system variables are measured at discrete spatial points and are not available over the complete range $0 \leq x \leq L$.

The unknown parameters are used to expand the system given by Eq. 21 from N dimensions to $(N+M)$ dimensions by noting that these parameters satisfy the differential equations

$$\underline{da}/dx = \underline{0} . \quad (24)$$

To obtain a solution for this expanded system it is necessary to provide at least M measurements to augment the boundary conditions given by Eq. 8. Often in actual systems the number of measurements exceed the number of unknown parameters, and some technique must be used to reduce the number of measurements to a useful form. The classical least-squares error criterion, consisting of a positive-definite functional Q based on the difference between the observed measurements $\underline{y}(x)$ and the calculated value $\underline{u}(x, \underline{a})$, is given by

$$Q = \sum_{j=1}^{M'} [\underline{y}(x_j) - \underline{u}(x_j, \underline{a})]^2 , \quad (25)$$

where

$$M' > M$$

and Q is minimized to obtain the M additional constraints.

The reason for using more measurements than are necessary is to distribute any discrepancies in the data to all points rather than relying on the values at a few points. A computational procedure for the identification problem is similar to the process already outlined for the system variables with the following additions. An initial approximation for $\underline{a}$ is made; the Jacobian matrix is of dimension $(N+M)$. The size of the $\underline{p}_{i+1}(x)$ vector is $(N+M)$, the $\underline{\psi}_{i+1}(x)$ matrix is $(N+M)$ by $(N-K+M)$, and the vector $\underline{\alpha}_{i+1}$ is of length $(N-K+M)$. To obtain the solution for $\underline{\alpha}_{i+1}$, the solution for $\underline{u}(x, \underline{a})$ in terms of $\underline{\alpha}_{i+1}$ is substituted into Eq. 25 and then minimized with respect to the M additional values of $\underline{\alpha}_{i+1}$. This result is combined

with Eq. 19 to obtain the solution for α_{i+1} , and the total solution for $u_{i+1}(x)$ and a are formed. The additional M values of α_{i+1} are the unknown parameters a . This iterative process is continued until a convergence criterion is satisfied.

F. Advantages and Disadvantages of Quasi-linearization

Because of the technique of imbedding the unknown a vector into the set of differential equations of the system, the identification process is limited to constant parameters. However, variable dependent coefficients can be obtained if they are written as functions of unknown and known mathematical functions, e.g., power series or polynomial approximations. Then the unknown constants in these expansions can be identified by the technique previously outlined.

The QL technique is an effective method for solving the identification problem in nonlinear models of lumped-parameter systems. It has the following advantages:

1. Solutions for linear and nonlinear systems are easily obtainable.
2. The numerical algorithm is easily programmable.
3. Convergence is quadratic in nature as the solution is approached.
4. Monotone convergence is obtained in many cases.

However, there are several drawbacks to the QL method:

1. Ultimate convergence is dependent upon a "good" initial estimate of the unknown variables and parameters.
2. No information about the unknown parameters is gained when the technique fails to converge.
3. A convergent solution may be obtained at a local minimum and not at the true values of the unknown parameters.

Many of these disadvantages can be overcome by combining the QL technique with other techniques outlined in Ch. I. Comparisons of these combined techniques have been shown to yield an improved algorithm^{20,21}. Numerical results for identification of a nonlinear, nuclear lumped-parameter model are presented in Ch. III.

III. PARAMETER IDENTIFICATION IN A NUCLEAR REACTOR SYSTEM

A. LMFBR Model

Numerical results of the parameter-identification technique developed in Ch. II have been obtained for reactor models involving one and two neutron-energy groups. The neutron-diffusion equations are coupled with thermal hydraulic equations to model the reactor core in the axial direction. The reactor model chosen for this analysis corresponds to a design of a liquid-metal fast breeder reactor (LMFBR).⁴⁶ In the axial direction, the reactor consists of three regions, a core of 165.81-cm height and two blanket regions, each of 45.72-cm height, for a total of 257.25 cm. Total reactor power is 2500 MWt, with 90% of the power being generated in the core. Fuel elements are composed of a mixture of uranium and plutonium oxides clad in stainless steel to provide a core power density of 400 kW/liter. Further reactor parameters for the LMFBR model are given in Appendix A.

Neutronic parameters were calculated by means of diffusion theory using the MACH-1 code.^{47,51} By this diffusion technique the reactor is treated as a slab or a one-dimensional cylinder with infinite transverse dimensions. The correction for the multidimensional reactor is accomplished by means of a transverse buckling term in the multigroup equations. Microscopic cross sections for the reactor were provided by the 26-group ANL-233 cross-section set. For the one- and two-neutron group models considered in this analysis, macroscopic cross sections were obtained by collapsing the multigroup values by a flux integral weighting technique, available as an option in the MACH-1 code.

B. One-neutron-energy-group Model

The first model to be investigated is that of one neutron-energy group with fuel and coolant temperature feedback. Equations for this model are

$$\frac{d\phi(x)}{dx} = -\frac{J(x)}{D(x)} ; \quad (26)$$

$$\begin{aligned} \frac{dJ(x)}{dx} = & \kappa \Sigma_o(x) \phi(x) + v \Sigma_f(x) \left\{ a_f \bar{\Delta T}_f(x) + a_c \Delta T_c(x) \right\} \\ & \times \phi(x) - \Sigma_a(x) \left\{ a'_f \bar{\Delta T}_f(x) + a'_c \Delta T_c(x) \right\} \phi(x) ; \end{aligned} \quad (27)$$

$$\frac{dT_c(x)}{dx} = \epsilon \Sigma_f(x) \phi(x) \left\{ 1 + a_f \bar{\Delta T}_f(x) + a_c \Delta T_c(x) \right\} ; \quad (28)$$

$$\bar{T}_f(x) = T_c(x) + \xi \Sigma_f(x) \phi(x) \{1 + a_f \Delta \bar{T}_f(x) + a_c \Delta T_c(x)\}; \quad (29)$$

$$\Delta T_c(x) = T_c(x) - T_c(0); \quad (30)$$

$$\Delta \bar{T}_f(x) = \bar{T}_f(x) - \bar{T}_f(0); \quad (31)$$

$$\bar{T}_f(0) = T_c(0), \quad (32)$$

where

- $\phi(x)$ - neutron flux,
- $J(x)$ - neutron current,
- $T_c(x)$ - coolant temperature,
- $\bar{T}_f(x)$ - average fuel temperature,
- $D(x)$ - diffusion coefficient,
- $\Sigma_a(x)$ - absorption cross section,
- $\Sigma_f(x)$ - fission cross section,
- ν - average number of neutrons per fission,
- $\Sigma_o(x)$ - $\nu \Sigma_f(x) - \Sigma_a(x)$,
- κ - criticality constant, indicating departure from criticality,
- a_f, a_c, a'_f, a'_c - temperature-feedback coefficients defined in Appendix A,
- ϵ, ξ - thermal-hydraulic parameters defined in Appendix A.

The variation in the fuel temperature, $\Delta \bar{T}_f(x)$, can be obtained in terms of $\Delta T_c(x)$ and $\phi(x)$ from Eqs. 29 through 32, i.e.,

$$\Delta \bar{T}_f(x) = \frac{\Delta T_c(x) + \xi \Sigma_f(x) \phi(x) [1 + a_c \Delta T_c(x)]}{1 - a_f \xi \Sigma_f(x) \phi(x)}. \quad (33)$$

The term $a_f \xi \Sigma_f(x) \phi(x)$ in the denominator of Eq. 33 is smaller by several orders of magnitude than one and the value of $\Delta \bar{T}_f(x)$ will be approximated by

$$\Delta T_f(x) \approx \Delta T_c(x) + \xi \Sigma_f(x) \phi(x) [1 + a_c \Delta T_c(x)] . \quad (34)$$

By using Eq. 34 in Eqs. 27 and 28 to eliminate $\Delta T_f(x)$, a new set of equations is obtained for the one-group model. To further simplify this model only the first-order terms of the feedback coefficients are kept in these equations. With values of the temperature-feedback coefficients of the order of 10^{-4} , there was only a 0.2% difference in the neutron flux between the results using the above approximations and those using Eq. 33 for $\Delta T_f(x)$. The equations for the one-neutron-energy-group model are now given by

$$\frac{d\phi(x)}{dx} = - \frac{J(x)}{D(x)} ; \quad (35)$$

$$\begin{aligned} \frac{dJ(x)}{dx} = & \kappa \Sigma_o(x) \phi(x) + \xi \Sigma_f(x) \left\{ a_f \nu \Sigma_f(x) - a'_f \Sigma_a(x) \right\} \\ & \times \phi^2(x) + \left\{ (a_f + a_c) \nu \Sigma_f(x) - (a'_f + a'_c) \right. \\ & \times \left. \Sigma_a(x) \right\} \phi(x) \Delta T_c(x) ; \end{aligned} \quad (36)$$

$$\frac{d\Delta T_c(x)}{dx} = \epsilon \Sigma_f(x) \phi(x) \left\{ 1 + \xi a_f \Sigma_f(x) \phi(x) + (a_f + a_c) \Delta T_c(x) \right\} . \quad (37)$$

As if all the coefficients of the above equations are specified, then three boundary conditions are necessary in order to obtain a solution for $\phi(x)$, $J(x)$, and $\Delta T_c(x)$. Usually, the neutron flux is assumed to be zero at the extrapolated boundaries of the reactor. The third condition can be obtained by specifying the coolant temperature at some position in the reactor. A convenient choice for $\Delta T_c(x)$ would be the value at the boundary of $x = 0$; a value of zero is chosen for $\Delta T_c(0)$. With these conditions, Eqs. 35 through 37 can be solved with the neutron flux and power level dependent on the values for the coefficients in these equations. If the desired power level is specified, it is necessary to consider one of the coefficients in the above equations as a variable to form a system of four equations and four boundary conditions. It is convenient to specify the criticality constant κ as an unknown variable which satisfies the differential equation

$$d\kappa/dx = 0 . \quad (38)$$

Typically, the reactor power is measured by the change in the coolant temperature across the reactor. Specifying $\Delta T_c(L)$ as 185°C corresponds to the total power of 2500 MWt, and this value will be used for the remainder of this analysis.

The LMFBR system is now modeled by a set of four nonlinear, ordinary differential equations, Eqs. 35 through 38, and four boundary conditions given by

$$\begin{aligned}
 \phi(0) &= 0 ; & \Delta T_c(0) &= 0 ; \\
 \phi(L) &= 0 ; & \Delta T_c(L) &= 185^\circ\text{C} .
 \end{aligned}
 \tag{39}$$

Due to the nonlinear nature of this two-point boundary-value problem, the QL technique will be employed to obtain the required values for the neutron flux, neutron current, coolant temperature change, and criticality constant κ . The solution of this problem illustrates the simplest identification problem and also provides the values for the simulated system measurements to be used in the identification of other system parameters.

C. Determination of Criticality Conditions

The solution of Eqs. 35 through 38 provides the criticality conditions for the LMFBR model. Coefficients of these equations are given in Table I, except for the values of the temperature feedback coefficients.

TABLE I. One-neutron-energy-group Coefficients

Parameter	Core	Blanket
D (cm)	1.0	1.0
Σ_a (cm ⁻¹)	5.446×10^{-3}	3.308×10^{-3}
Σ_f (cm ⁻¹)	1.9445×10^{-3}	2.2241×10^{-4}
$\nu\Sigma_f$ (cm ⁻¹)	5.7945×10^{-3}	5.7827×10^{-4}
ϵ (°C-cm ² -sec)	1.1448×10^{-13}	1.1448×10^{-13}
ξ (°C-cm ³ -sec)	9.391×10^{-11}	9.391×10^{-11}

With these values for the coefficients, a set of κ values will be determined to correspond to various values of temperature-feedback coefficients. To determine the zero feedback value of κ , the temperature-feedback coefficients are set equal to zero. Although the system equations now appear to be linear, the model remains nonlinear, since κ is a system variable and the term $\kappa\Sigma_o(x)\phi(x)$ appears in Eq. 36. The solution of this no-feedback case will be used to illustrate the QL procedure developed in Sect. II.C.

Equations 35 through 38 are in the form of Eq. 7; the system variable vector $\underline{u}(x)$ is given by

$$\underline{u}(x) = \begin{bmatrix} \phi(x) \\ J(x) \\ \Delta T_c(x) \\ \kappa \end{bmatrix} , \tag{40}$$

and the vector function $\underline{F}[\underline{u}(x), x]$ is given by

$$\underline{F}[\underline{u}(x), x] = \begin{bmatrix} -\frac{J(x)}{D(x)} \\ \kappa \Sigma_o(x) \phi(x) \\ \epsilon \Sigma_f(x) \phi(x) \\ 0 \end{bmatrix}. \quad (41)$$

Boundary conditions given by Eq. 39 satisfy the general boundary-condition matrix, Eq. 9. The initial estimate for $\underline{u}(x)$ is based on a $\sin(\pi x/L)$ shape for $\phi(x)$, a $\cos(\pi x/L)$ shape for $J(x)$, and a $[1 - \cos(\pi x/L)]$ shape for $\Delta T_c(x)$. The initial estimate for κ is unity. These values are then used to evaluate the Jacobian matrix:

$$\underline{H}(\underline{u}) = \begin{bmatrix} 0 & -\frac{1}{D(x)} & 0 & 0 \\ \kappa \Sigma_o(x) & 0 & 0 & \Sigma_o(x) \phi(x) \\ \epsilon \Sigma_f(x) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \quad (42)$$

The solution of the quasi-linearized Eq. 10 is obtained by superposition, using the solutions for the particular solution vector $\underline{p}_{i+1}(x)$, Eq. 14, and the homogeneous solution matrix $\underline{\psi}_{i+1}(x)$, Eq. 15. By use of these results the matrix 19 is solved for the values of $\underline{\alpha}_{i+1}$, which are $J(0)$ and κ for this problem. The solution for the system variables is now formed by using Eq. 13. Values obtained from this solution are compared with the initial estimates using the convergence criterion, Eq. 6 with $\mu = 10^{-6}$. If the convergence criterion is not satisfied, the values obtained from this iteration are used as the new approximations for the system variables. The Jacobian matrix is evaluated using these new values, and a new solution using the technique of superposition is obtained. This process is repeated until the convergence criterion is satisfied.

Convergence for the zero-feedback case was obtained in five iterations, giving $\kappa = 0.650673$. Values of κ at the end of each iterative cycle are given in Table II. Computational time for this problem was 11 sec with the IBM-360 Model 50/75 computer; the differential equations were solved by finite-differencing technique using 101 spatial mesh points.

TABLE II. κ Values at End of Each Iterative Cycle

Iteration No.	κ Value
0	1.0
1	0.62704
2	0.652017
3	0.650674
4	0.650673
5	0.650673

A flow chart for the criticality problem is given by Fig. 2. The value $\mu = 10^{-6}$ was chosen for all problems solved by the QL procedure; the maximum number of iterations, $i_{\max}$, was arbitrarily chosen to be 15. To integrate the system differential equations numerically, a finite-difference formulation was made and a fourth-order Runge-Kutta⁴⁸ routine was chosen for all the calculations. Several values for the spatial mesh spacings were chosen, but calculations indicated that the accuracy of the results was not increased significantly if more than 101 mesh points were used. For the solution of the linear algebraic equations given by Eq. 19, a modified Gaussian elimination technique was employed. This technique, known as the Crout routine,⁴⁹ employs partial pivoting to improve the solution of the matrix equations.

To illustrate the effect of the temperature feedback on the neutron flux and temperature shapes, the feedback coefficients were chosen to be 10^{-4} . Initial estimates for $u(x)$ were based on the results of the no-feedback model. A comparison of the feedback and no-feedback models are shown in Fig. 3. The neutron flux, and the fuel and coolant temperature changes for the no-feedback model are given by the dashed lines, and for the feedback case by the solid lines. Results for this one-neutron-energy-group model were reported by Habegger and Hsu.²⁷ Determination of criticality conditions is essential for future identification problems. Results of the criticality problem are used to obtain the simulated measurements to be used in the identification of system parameters.

D. Identification of Two Temperature-feedback Coefficients

The determination of the temperature-feedback coefficients will be used to illustrate parameter identification by the QL technique. In order to determine these parameters, additional conditions are necessary to augment the boundary conditions given by Eq. 39. These additional conditions will be obtained by simulated measurements of the reactor system variables that were calculated by the determination of the criticality conditions. The first example of determining temperature-feedback coefficients will be the determination of two coefficients a_f and a_c in Eqs. 36 and 37. The values for a_f' and a_c' are specified as zero. This choice retains the non-linear terms in both Eqs. 36 and 37. Equation 36 is now written as

Fig. 2. Flow Chart for Criticality Problem.

Fig. 3. Comparison of Feedback and No-feedback Models for One Neutron-energy Group.

$$\begin{aligned} \frac{dJ(x)}{dx} = & \kappa \Sigma_0(x) \phi(x) + \xi a_f \nu \Sigma_f^2(x) \phi^2(x) \\ & + (a_f + a_c) \nu \Sigma_f(x) \phi(x) \Delta T_c(x) . \end{aligned} \quad (43)$$

In order to obtain values for the feedback coefficients a_f and a_c , EBR-II design parameters⁵⁰ were modified to obtain values for this particular model. The values chosen for the coefficients were

$$\begin{aligned} a_f &= -0.4 \times 10^{-5}/^{\circ}\text{C} ; \\ a_c &= -0.2 \times 10^{-4}/^{\circ}\text{C} . \end{aligned}$$

With these values the criticality constant κ was determined by the technique of Sect. III.C. The calculated value of κ was 1.2817. To identify the fuel and coolant temperature coefficients the following differential equations:

$$\frac{da_f}{dx} = 0 ; \quad \frac{da_c}{dx} = 0 , \quad (44)$$

were combined with Eqs. 35, 37, and 43 to provide the system equations. In addition to the boundary conditions, Eq. 39, one additional condition or constraint is obtained to solve the set of five differential equations.

From a set of simulated neutron-flux measurements which are available from the solution of the criticality conditions, the additional constraint is chosen to be the minimization of the following function:

$$Q_1 = \sum_{j=1}^{M'} [y(x_j) - \phi(x_j)]^2, \quad (45)$$

where M' is the number of simulated neutron-flux measurements, $y(x_j)$ is the neutron-flux value at point x_j obtained from the criticality solution, and $\phi(x_j)$ is the calculated neutron flux obtained from the solution of the system equations. An arbitrary choice of nine neutron-flux values ($M' = 9$) were selected at equally spaced points throughout the blanket and core regions of the reactor.

Initial estimates for a_f and a_c were chosen to be $-0.2 \times 10^{-5}/^{\circ}\text{C}$ and $-0.1 \times 10^{-4}/^{\circ}\text{C}$, respectively, which are 50% less than the true values. The initial estimates for the system variables were based on the results of the no-feedback case. With these initial estimates and the nine simulated neutron-flux measurements, a convergent solution was obtained in six iterations. The identified values for a_f and a_c were $-0.399839 \times 10^{-5}/^{\circ}\text{C}$ and $-0.198235 \times 10^{-4}/^{\circ}\text{C}$, which are in error from the true values by 0.04% and 0.9%, respectively.

Further studies were made to establish a range of convergence when the initial estimates of the temperature-feedback coefficients were varied, but no definite range could be determined. Convergent solutions were obtained even when initial estimates of a_f and a_c were in error by several orders of magnitude.

The number of spatial mesh points used in the numerical evaluation of the system equations was 101, the same as the number used in the determination of the criticality conditions. Computational time for the identification of a_f and a_c was approximately 2 sec per iteration. Increasing the number of mesh points yielded an insignificant increase in the accuracy of the identification of a_f and a_c , whereas the computational time per iteration doubled as the number of mesh points were doubled. Further studies revealed that use of less than 101 mesh points made no significant change in the accuracy of the identification. However, reducing the mesh spacings below 51 significantly changed the values of the system variables and identified parameters.

1. Effect of Number and Accuracy of Measurements on Identification. The selection of nine measurements of neutron flux was chosen arbitrarily, and a study was made on the effect of increasing or decreasing this number. Increase from nine to nineteen yielded a very slight increase (0.01%) in the accuracy of the identification of a_f and a_c . Decrease to five yielded only a slight decrease in the accuracy of determining the temperature-feedback coefficients. However, when the number of measurements was reduced further to three, there was a doubling of the error in the determination of a_c to 2%; the accuracy of the identification of a_f decreased but slightly. These studies were made with initial values for a_f

and a_c 50% less than the true values, and with the initial values of the system variables given by the results of the no-feedback model.

The next step was to reduce the number of measurements to one; thus, the additional condition was supplied by specifying the neutron flux at a single position in the reactor. When the above initial estimates of the system variables and unknown parameters were used, a convergent solution was not obtained. Reducing the error in the initial estimates to within 25% of the true values still failed to yield a solution. A convergent solution was obtained when the true values of a_f and a_c were used as the initial parameter estimates with the initial system variable estimates still based on the results of the no-feedback model. The results obtained from this analysis were $a_f = -0.400005 \times 10^{-5}/^{\circ}\text{C}$ and $a_c = -0.199976 \times 10^{-4}/^{\circ}\text{C}$. Similar results were obtained when the single neutron-flux measurement was made at various positions in the reactor.

Measurement values used in the previous analysis were based on values that were in error by less than $10^{-4}\%$. Actual neutron-flux measurements in a reactor system cannot be obtained to this accuracy. Therefore, a study was made to determine the effect of reducing the accuracy of the measurements on the identification of a_f and a_c . Measurement errors were increased approximately to 0.1% and 1%; the results of this analysis are given in Table III.

TABLE III. Effect of Measurement Error on the Accuracy of Identification

Measurement Error:	$10^{-4}\%$	0.1%	1.0%
$a_f (10^5) (^{\circ}\text{C}^{-1})$	-0.399839	-0.400358	-0.395024
% error in a_f	0.0403	0.0895	1.24
$a_c (10^4) (^{\circ}\text{C}^{-1})$	-0.198235	-0.193881	-0.23864
% error in a_c	0.883	3.06	19.3
$Q_1 (10^5)$	0.16795	0.17781	3.2024

When the accuracy of the measurements is decreased there is a significant increase in the error in determining a_c as compared with the increase in the error of identifying a_f . This effect is attributed to the fact that the feedback effect provided by the fuel-temperature coefficient a_f was greater by several orders of magnitude than the effect of the coolant-temperature coefficient a_c . This dominance of a_f over a_c occurred when an error was made in the formulation of the reactor model when the neutron flux and coolant temperatures were normalized. The results in Table III show that an increase in the measurement error decreases the accuracy of the identification of the less dominant coefficient a_c significantly. As noted earlier, a similar result occurred in identifying a_c when the number of measurements were decreased from nine to three.

2. Effect of Magnitude of Parameters and Criterion Function on Identification. The accuracy of the identification of the temperature-feedback coefficients is increased as the system becomes more nonlinear, since a_f and a_c are the coefficients of the nonlinear terms. Results of this analysis are given in Table IV.

TABLE IV. Accuracy of Identification Based on the Magnitude of the Feedback Coefficients

	Case 1	Case 2
$a_f(10^6) (^{\circ}\text{C}^{-1})$	-0.401262	-4.00058
% error a_f	0.313	0.0145
$a_c(10^4) (^{\circ}\text{C}^{-1})$	-0.39868	-3.99627
% error a_c	0.33	0.093
κ value	0.793440	1.97192
$Q_1(10^5)$	0.150126	0.199326

In the first case, a_f was chosen to be $-0.4 \times 10^{-6}/^{\circ}\text{C}$ and a_c a hundred times larger, so that the feedback effects of the fuel and coolant temperature changes were approximately equal. For the second case, the values of a_f and a_c were increased by a factor of ten.

The criterion function is now modified to include both neutron-flux and coolant-temperature measurements. The function to be minimized is given by

$$Q_2 = \sum_{j=1}^{M'} [y(x_j) - \phi(x_j)]^2 + \sum_{k=1}^{R'} [z(x_k) - \Delta T_c(x_k)]^2, \quad (46)$$

where R' is the number of simulated measurements of coolant temperature change, $z(x_k)$ is the coolant temperature change at point x_k obtained from the criticality solution, and $\Delta T_c(x_k)$ is the calculated value from the solution of the system equations. Nine measurements were employed for both the neutron flux ($M' = 9$) and coolant temperature change ($R' = 9$). With these values and the initial estimate of a_f and a_c being 50% less than the true values, a convergent solution was obtained in six iterations. The identified values were $a_f = -0.399711 \times 10^{-5}/^{\circ}\text{C}$ and $a_c = -0.199307 \times 10^{-4}/^{\circ}\text{C}$, with $Q_2 = 0.168287 \times 10^{-5}$. There is an increase in the accuracy of identifying a_c when compared with the results using only neutron flux measurements, while a very slight decrease occurred in identifying a_f .

Another modification was made to the criterion function to study the effect on the identification of the unknown parameters. The system boundary conditions, Eq. 39, are now considered as measurements and are added to the Q_1 criterion function. The new criterion function to be minimized is given by

$$Q_3 = \sum_{j=1}^{M'} [y(x_j) - \phi(x_j)]^2 + W_1 [\phi^2(0) + \phi^2(L)]^2 + W_2 [\Delta T_c^2(0) + (185^\circ\text{C} - \Delta T_c[L])^2] , \quad (47)$$

where W_1 and W_2 are weighting constants that specify the worth of the boundary values in the minimization process. As the values of W_1 and W_2 are increased the results obtained from using the Q_3 criterion function will approach the results obtained from using Q_1 . Table V gives the results for identifying a_f and a_c as the values of W_1 and W_2 are varied. There is an increase in the accuracy of the identification when the boundary conditions are treated as measurements since the identification process is less dependent on satisfying the boundary values and is based more on satisfying the neutron-flux shape given throughout the core. As anticipated the results for large values of W_1 and W_2 are the same as those obtained using Q_1 .

TABLE V. Effect of Equal Values of W_1 and W_2 on the Accuracy of the Parameter Identification

W_1, W_2	1.0	10	10^2	10^3	10^4
$a_f (10^5)$	-0.399914	-0.399853	-0.399841	-0.399841	-0.399839
% error a_f	0.0215	0.0368	0.0398	0.0403	0.0403
$a_c (10^4)$	-0.199268	-0.198430	-0.198257	-0.198237	-0.198235
% error a_c	0.366	0.785	0.872	0.882	0.883
$Q_3 (10^6)$	0.799506	1.37798	1.64330	1.6759	1.67911
$Q_1 (10^6)$	0.380705	1.36299	1.64312	1.67579	1.67911

E. Identification of Four Temperature Feedback Coefficients

To determine the additional feedback coefficients of a'_f and a'_c the following differential equations:

$$\frac{da'_f}{dx} = 0 ; \quad \frac{da'_c}{dx} = 0 , \quad (48)$$

are added to Eqs. 35 through 37 and 44 to describe the behavior of the system. Values for the feedback coefficients were chosen to be⁵¹

$$a_f = -0.4 \times 10^{-5}/^\circ\text{C};$$

$$a_c = -0.2 \times 10^{-4}/^\circ\text{C};$$

$$\begin{aligned} a'_f &= +0.4 \times 10^{-6}/^{\circ}\text{C}; \\ a'_c &= -0.4 \times 10^{-5}/^{\circ}\text{C}. \end{aligned}$$

An initial estimate of $-0.1 \times 10^{-5}/^{\circ}\text{C}$ was made for each of the unknown parameters, and both Q_1 and Q_2 functions were used in the minimization process. The error in the normalization of the flux and coolant temperature variables that was present in the two-parameter identification was corrected for this analysis. Convergent solutions were obtained in eight iterations using Q_1 and in five iterations using Q_2 . Results of the identification of the four feedback coefficients are given in Table VI. The values for the system variables obtained with these feedback coefficients will be used for the initial conditions of the distributive-parameter reactor model identification of Ch. V.

TABLE VI. Identification of Four Temperature Coefficients

	Q_1	Q_2
$a_f(10^5)(^{\circ}\text{C}^{-1})$	-0.400001	-0.399977
$a_c(10^4)(^{\circ}\text{C}^{-1})$	-0.199996	-0.200017
$a'_f(10^6)(^{\circ}\text{C}^{-1})$	+0.400011	+0.40024
$a'_c(10^5)(^{\circ}\text{C}^{-1})$	-0.399962	-0.400179
$Q_1(10^{12})$	0.175076	-
$Q_2(10^{10})$	-	0.469161

Further analysis of the four-parameter identification problem based on varying the magnitudes of the feedback coefficients yielded similar results in the accuracy of the identification. The next problem will be modeling of the reactor by a two-neutron-energy-group model.

F. Two-neutron-energy-group Model

A two-neutron-energy-group model will now be examined to determine criticality conditions and to identify fuel and coolant temperature coefficients. The two-group parameters were obtained by using the group-collapsing technique of the MACH-1 diffusion code.⁴⁷ Determinations of the fast and slow groups were made by selecting the four highest energy groups in the ANL-233 26-group set of cross sections as the fast group. The average neutron velocity for this fast group is 1.92×10^9 cm/sec; the average neutron velocity for the slow group is 1.99×10^8 cm/sec. The following equations represent the two-neutron-energy-group model:

$$\frac{d\phi_1}{dx} = \frac{J_1(x)}{D_1(x)}; \quad (49)$$

$$\begin{aligned}
\frac{dJ_1(x)}{dx} &= -\kappa \Sigma_{c_1}(x) \phi_1(x) - \Sigma_{12} \phi_1(x) \\
&+ \chi_1 v_1 \Sigma_{f_1}(x) \phi_1(x) + \chi_1 v_2 \Sigma_{f_2}(x) \phi_2(x) \\
&+ [\chi_1 v_1 \Sigma_{f_1}(x) \phi_1(x) + \chi_1 v_2 \Sigma_{f_2}(x) \phi_2(x)] \cdot \\
&\times \left\{ a_f^* \Delta \bar{T}_f(x) + a_c^* \Delta T_c(x) \right\} ; \quad (50)
\end{aligned}$$

$$\frac{d\phi_2(x)}{dx} = - \frac{J_2(x)}{D_2(x)} ; \quad (51)$$

$$\begin{aligned}
\frac{dJ_2(x)}{dx} &= -\kappa \Sigma_{c_2}(x) \phi_2(x) + \Sigma_{12}(x) \phi_1(x) \\
&+ \chi_2 v_1 \Sigma_{f_1}(x) \phi_1(x) + \chi_2 v_2 \Sigma_{f_2}(x) \phi_2(x) \\
&+ [\chi_2 v_1 \Sigma_{f_1}(x) \phi_1(x) + \chi_2 v_2 \Sigma_{f_2}(x) \phi_2(x)] \\
&\times \left\{ a_f^* \Delta \bar{T}_f(x) + a_c^* \Delta T_c(x) \right\} ; \quad (52)
\end{aligned}$$

$$\begin{aligned}
\frac{dT_c(x)}{dx} &= \varepsilon [\Sigma_{f_1}(x) \phi_1(x) + \Sigma_{f_2}(x) \phi_2(x)] \\
&\times \left\{ 1 + a_f^* \Delta \bar{T}_f(x) + a_c^* \Delta T_c(x) \right\} ; \quad (53)
\end{aligned}$$

$$\begin{aligned}
\bar{T}_f(x) &= T_c(x) + \xi [\Sigma_f(x) \phi_1 + \Sigma_{f_2}(x) \phi_2(x)] \\
&\times \left\{ 1 + a_f^* \Delta \bar{T}_f(x) + a_c^* \Delta T_c(x) \right\} , \quad (54)
\end{aligned}$$

where

- $1, 2$ - subscripts referring to fast and slow groups, respectively,
 D_i - diffusion coefficient of i^{th} group,
 ϕ_i - neutron flux of i^{th} group,
 J_i - neutron current of i^{th} group,
 Σ_{ci} - capture cross section for i^{th} group,
 Σ_{fi} - fission cross section for i^{th} group,
 Σ_{12} - scattering cross section from group 1 to group 2,
 ν_i - average number of neutrons produced by fission for group i ,
 χ_i - fraction of neutrons born in group i ($\chi_1 + \chi_2 = 1$).

The criticality constant κ has been slightly redefined from the one-group case in that it multiplies only the capture cross sections in both groups instead of the total cross section as in the one-group case. Also, the feedback coefficients a_f^* and a_c^* have been redefined to simplify the model, and again the feedback effect will be limited to the fission cross section only. As was done for the one-group case, the system equations are simplified and combined into the following set of equations:

$$\frac{d\phi_1}{dx} = -\frac{J_1(x)}{D_1(x)} ; \quad (55)$$

$$\begin{aligned}
 \frac{dJ_1(x)}{dx} = & -\kappa \Sigma_{c1}(x) \phi_1(x) - \Sigma_{12} \phi_1(x) + \chi_1 \nu_1 \Sigma_{f1}(x) \phi_1(x) \\
 & + \chi_1 \nu_2 \Sigma_{f2}(x) \phi_2(x) + [\chi_1 \nu_1 \Sigma_{f1}(x) \phi_1(x) \\
 & + \chi_1 \nu_2 \Sigma_{f2}(x) \phi_2(x)] \{ [a_f^* + a_c^*] \Delta T_c(x) \\
 & + a_f^* \xi [\Sigma_{f1}(x) \phi_1(x) + \Sigma_{f2}(x) \phi_2(x)] \} ; \quad (56)
 \end{aligned}$$

$$\frac{d\phi_2(x)}{dx} = -\frac{J_2(x)}{D_2(x)} ; \quad (57)$$

$$\begin{aligned}
\frac{dJ_2(x)}{dx} = & -\kappa \Sigma_{c_2}(x) \phi_2(x) + \Sigma_{12}(x) \phi_1(x) + \chi_2 \nu_1 \Sigma_{f_1}(x) \phi_1(x) \\
& + \chi_2 \nu_2 \Sigma_{f_2}(x) \phi_2(x) + [\chi_2 \nu_1 \Sigma_{f_1}(x) \phi_1(x) \\
& + \chi_2 \nu_2 \Sigma_{f_2}(x) \phi_2(x) \{ [a_f^* + a_c^*] \Delta T_c(x) \\
& + a_f^* \xi [\Sigma_{f_1}(x) \phi_1(x) + \Sigma_{f_2}(x) \phi_2(x)] \} ; \quad (58)
\end{aligned}$$

$$\begin{aligned}
\frac{d\Delta T_c(x)}{dx} = & \epsilon [\Sigma_{f_1}(x) \phi_1(x) + \Sigma_{f_2}(x) \phi_2(x)] \\
& \times \left\{ 1 + (a_f^* + a_c^*) \Delta T_c(x) + a_f^* \xi [\Sigma_{f_1}(x) \phi_1(x) \right. \\
& \left. + \Sigma_{f_2}(x) \phi_2(x)] \right\} . \quad (59)
\end{aligned}$$

With these five equations, the criticality conditions can be obtained by solving for κ by adding the differential equation

$$\frac{d\kappa}{dx} = 0 . \quad (60)$$

Boundary conditions for this set of equations are given by

$$\begin{aligned}
\phi_1(0) &= 0 ; & \phi_1(L) &= 0 ; \\
\phi_2(0) &= 0 ; & \phi_2(L) &= 0 ; \\
\Delta T_c(0) &= 0 ; & \Delta T_c(L) &= 185^\circ\text{C} . \quad (61)
\end{aligned}$$

The system coefficients are given in Table VII.

TABLE VII. Two-neutron-energy-group Coefficients

Parameter	Core	Blanket
D_1 (cm)	3.20178	3.27137
D_2 (cm)	1.35672	1.25
Σ_{c_1} (cm ⁻¹)	5.03008×10^{-3}	3.68209×10^{-3}
Σ_{c_2} (cm ⁻¹)	4.79576×10^{-3}	3.71997×10^{-2}
Σ_{12} (cm ⁻¹)	3.08346×10^{-2}	3.11396×10^{-2}
Σ_{f_1} (cm ⁻¹)	4.47460×10^{-3}	3.15689×10^{-3}
Σ_{f_2} (cm ⁻¹)	1.75471×10^{-3}	8.71051×10^{-3}
ν_1	2.97553	2.80387
ν_2	2.90273	2.86442
χ_1	0.5604	0.5604
χ_2	0.4396	0.4396
ϵ (°C-cm ² -sec)	1.1448×10^{-13}	1.1448×10^{-13}
ξ (°C-cm ³ -sec)	9.391×10^{-11}	9.391×10^{-11}

Results for the no-feedback case yielded a criticality value $\kappa = 1.13126$ in four iterations when the initial estimate of 1.0 was made for κ . Computational time was approximately 4 sec per iteration using 101 mesh points in the numerical integration. The solution of the criticality problem will be used to obtain the simulated neutron-flux values used in the identification problem.

To identify the feedback coefficients the following differential equations:

$$\frac{da_f^*}{dx} = 0, \quad \frac{da_c^*}{dx} = 0, \quad (62)$$

are combined with Eqs. 55 through 59. In addition to the boundary conditions, Eq. 61 the following criterion function is used:

$$Q_4 = \sum_{j=1}^{M'} [y(x_j) - \phi_1(x_j) - \phi_2(x_j)]^2, \quad (63)$$

where $y(x_j)$ is the sum of the values of the fast- and slow-neutron fluxes at point x_j obtained from the criticality solution. The total neutron flux is now used in the minimization of the criterion function.

Two cases were analyzed to illustrate the identification of parameters for two neutron energy groups: for the first case values of $-1.0 \times 10^{-4}/^{\circ}\text{C}$ were chosen for a_f^* and a_c^* ; for the second case values were increased by a factor of ten. With the initial estimates in error by 200% of the true values and nine flux measurements, convergent solutions were obtained in six iterations for both cases. Results of these cases are given in Table VIII.

TABLE VIII. Identification of Temperature Coefficients in Two-neutron-energy-group Model

	Case 1	Case 2
$a_f (10^4) (^{\circ}\text{C}^{-1})$	-0.99844	-9.99813
% error a_f	0.156	0.0187
$a_c (10^4) (^{\circ}\text{C}^{-1})$	-1.0022	-1.00017
% error a_c	0.22	0.017
$Q_1 (10^{11})$	0.410000	0.549851

G. Discussion of Results and Conclusions

The quasi-linearization technique has been shown to be an effective method for identifying parameters in a nonlinear nuclear reactor system. Identification of up to four temperature coefficients in a one-neutron-energy-group model and two coefficients in a two-group model has been shown to yield excellent results. In addition to demonstrating the applicability of the QL technique to reactor system models, various formulations of the identification problem were studied.

Solutions were obtained for two and four temperature-feedback coefficients when nine simulated neutron-flux measurements were used with initial parameter estimates that were in error by at least 50% from the actual values. Further studies using these nine measurements in identifying two parameters showed that solutions are obtainable even when the initial estimates of the parameter values were in error by two orders of magnitude from the actual values. Based on these results and the fact that in practice some knowledge of the physical system will usually yield estimates within one order of magnitude, the determination of the region of convergence was not pursued further. When the number of simulated neutron-flux measurements were varied, the accuracy of the identification increased as the number of measurements increased. Results of this analysis indicated that a threshold number exists such that the accuracy of the identification increases insignificantly as the number of measurements increases past this threshold. For equally spaced measurements throughout the reactor, there was only a slight increase in accuracy when more than five measurement values were used in the least-squares criterion.

When errors were introduced in the measurement values, the accuracy of the identification predictably decreased. The relationship between measurement error and identification error is proportional to the effect each parameter has on the system. The greatest error in the identification occurred for the less dominant parameter. Results also showed that the accuracy of the identification for the temperature-feedback coefficients increased as their magnitudes increased, which corresponds to the system being more nonlinear.

The use of additional information in the criterion function resulted in less error in the identification of the unknown parameters. When coolant temperature measurements were added to the criterion function, the accuracy of identifying the coolant temperature coefficient increased. This parameter is the coefficient of the nonlinear terms that vary as the coolant temperature changes. Increased accuracy occurred when the system boundary conditions were considered as measurements and were incorporated into the criterion function. The increase in identification accuracy resulted from the fact that the identification process is less dependent on the boundary values and is based more on the neutron-flux shape throughout the core. Neutron-flux values near the boundaries of the reactor are smaller by several orders of magnitude than the centerline values, and thus failing to satisfy these values has very little effect on the analysis of the reactor, but does increase the accuracy of parameter identification.

Computational time on the computer was very small for each iteration and the number of iterations were reduced due to the excellent convergent properties of the QL technique. The QL technique transformed the original multipoint boundary-value problem into a set of initial-value problems which are solved more efficiently on the computer.

Although this analysis was limited to mathematical models of a nuclear reactor system, the extension to parameter identification based on experimental results is feasible. The properties exhibited by the QL technique of rapid convergence, large region of convergence, and few measurements to obtain accurate identification form the basis for its application to experimental analysis. Also the QL technique can be extended to predict the methods of performing the experiment. Then mathematical analysis can be utilized to determine the position of detectors, the number of measurements required, and the variables to be measured. Finally, the results of this analysis are used to furnish the steady-state conditions for the time-dependent nuclear reactor model discussed in Ch. V.

IV. DISTRIBUTIVE-PARAMETER IDENTIFICATION

A. Introduction

Previously, the quasi-linearization procedure was shown to be an effective method of solving the problem of lumped-parameter identification. To apply the QL procedure to distributive-parameter systems poses additional computational difficulties. Initially, the partial differential equations are quasi-linearized and then solved by a standard numerical technique for linear partial differential equations. This process continues iteratively until a convergent solution is obtained. Bellman and Kalaba¹⁸ outline this technique for nonlinear parabolic, hyperbolic, and elliptic partial differential equations. The added difficulties arise in formulating the solution by use of superposition. Previously, for ordinary differential equations, an arbitrary choice for the missing conditions at $x = 0$ was made to obtain the homogeneous and particular solutions. For distributive-parameter systems, missing conditions may exist not only at the spatial boundaries, but also for the initial conditions at zero time. It has been shown⁵² that in order to utilize superposition to solve the distributive system, a specific choice for the unknown conditions must be made in order to obtain a convergent solution.

To extend the QL technique to the problem of distributive-parameter identification, it is necessary to write the additional partial differential equations for the unknown parameters:

$$\frac{\partial \underline{a}}{\partial x} = 0 ; \quad \frac{\partial \underline{a}}{\partial t} = 0 . \quad (64)$$

These equations stipulate that the unknown parameters $\underline{a}$ are constant with respect to both the spatial and temporal behavior of the system. In order to solve numerically the system of partial differential equations including Eq. 64, it is necessary to construct a massive set of algebraic equations by finite differencing the original partial derivatives in both space and time. The computation problems of solving this enormous set of algebraic equations make this approach unsuitable.

The alternative approach^{53,54} of finite differencing the partial derivatives with respect to only one of the independent variables also causes difficulty in the identification process. By finite differencing only a single set of partial derivatives, a set of differential difference equations are formed which can be solved by the QL techniques outlined earlier in Ch. II. With this approach only one additional equation need now be given for each of the unknown parameters. But it is now necessary to solve iteratively the system equations at each of the discretized points and, therefore, measurement values must be given for each of these points. Often it is impossible physically to obtain values for each of the mesh points since the finite-differencing technique may require very small mesh spacings in order to obtain the desired numerical accuracy.

Due to the difficulties of adapting the quasi-linearization procedure to the distributive-parameter problem, an alternative technique will be employed to solve the identification problem. Before discussing this technique, the distributive-parameter system model will be described. The discussion of the selected techniques will be given in Sect. IV.C.

B. Distributive-parameter Model and Criterion Function

The distributive-parameter system will be assumed to be modeled by a set of N partial differential equations of the form

$$\frac{\partial \underline{u}(x,t)}{\partial t} = \underline{F} \left(x, t, \underline{u}, \frac{\partial \underline{u}}{\partial x}, \frac{\partial^2 \underline{u}}{\partial^2 x}, \underline{a} \right), \quad (65)$$

where $\underline{u}(x,t)$ and $\underline{F}(\dots)$ are an N -dimensional column vector and vector function, respectively. Equation 65 is a valid description of both parabolic and hyperbolic partial differential equations. The unknown parameters to be identified are given by the M -dimensional vector $\underline{a}$. Initial conditions for the system of equations are given by

$$\underline{u}(x,0) = \underline{u}_0(x) \quad (66)$$

with boundary conditions at $x = 0$ given by

$$\underline{\alpha} \left(\frac{\partial \underline{u}}{\partial x}, \underline{u}, t \right) = 0 \quad (67)$$

and at $x = L$ by

$$\underline{\beta} \left(\frac{\partial \underline{u}}{\partial x}, \underline{u}, t \right) = 0. \quad (68)$$

It would be possible to include the unknown parameter vector $\underline{a}$ in the initial and boundary conditions, but this will not be considered for this analysis. Equations 67 and 68 are valid for all time greater than zero ($t > 0$), whereas Eq. 66 is valid over all space ($0 < x < L$).

Since there are M unknown parameters, it is necessary to provide at least M additional conditions to solve the identification problem. These conditions are obtained from measurements, $\underline{y}(x,t)$, of the system which can be either space- or time-dependent or both. The measured values will be obtained at discrete values of space and time, and it will also be assumed that the system variables, $\underline{u}(x,t)$, are directly measureable. A least-squares error criterion will be employed as the criterion function to be minimized. It is based on the difference between the measurement values, $\underline{y}(x,t)$, and the calculated values, $\underline{u}(x,t)$, at the discrete values (x_r, t_s) . The criterion function Q is given by

$$Q = \sum_{r=1}^R \sum_{s=1}^S [y(x_r, t_s) - \underline{u}(x_r, t_s)]^2, \quad (69)$$

where RS is the total number of measurement values. It is also assumed that N' of the system variables are measured, where $N' \leq N$.

There are numerous variations of the above problem, and in general the techniques presented in this chapter are easily modified for these problems. It has been shown¹³ that many types of criterion functions are, in general, variations of the least-squares criterion with different weighting functions. In this analysis the weighting function in Eq. 69 was chosen for convenience as unity to give equal importance for all measurements in the minimization of the criterion function.

C. Parameter Identification and Gradient Techniques

A parameter-identification technique must be capable of proceeding from an initial estimate of the unknown parameters to some value which makes the system-model solution approach the actual system-output measurements. For the distributive-parameter system the degree of similarity between the model and the measurements is determined by the criterion function, Eq. 69. Thus, the values of $\underline{a}$ that minimize the criterion function can be considered to be the solution of the identification problem. By regarding the identification problem as a problem of function minimization, it is possible to take advantage of the recent advances made in this area.^{7,11,12}

The specific minimization techniques to be examined for distributive-parameter identification are the gradient methods. These methods derive their name from the fact that the upgrading of the initial estimate of the unknown parameters is based on the information provided by the slope of the criterion function with respect to the unknown parameters. Originally, gradient techniques were developed to locate the minimum of an algebraic function. They will now be extended to the minimization of the criterion function subject to the constraints of the governing system equations. Initial work in using gradient methods for distributive-parameter systems was done by Seinfeld³⁷ and Herbold.³⁸

In this analysis, gradient search directions are defined as any search directions whose components are related to the values of $\partial Q / \partial \underline{a}$. All of the gradient methods are based on an iterative procedure that determines the (i+1) iterative value of $\underline{a}$ from a known $\underline{a}_i$ value by the following relation:

$$\underline{a}_{i+1} = \underline{a}_i + \rho_i \underline{d}_i, \quad (70)$$

where $\underline{d}_i$ is an M-dimensional search direction vector selected by using the information known about the system parameters, criterion function, and gradient of the criterion function at the i^{th} iteration. The specific choice of $\underline{d}_i$ depends upon the gradient technique being employed. The scalar ρ_i is the distance moved along the direction $\underline{d}_i$, and the value of ρ_i is chosen to satisfy the inequality

$$Q(\underline{a}_{i+1}) < Q(\underline{a}_i) , \quad (71)$$

where $Q(\underline{a}_i)$ is the value of the criterion function, Eq. 69, for the i^{th} iterative value of the unknown parameters. Satisfying Eq. 71 insures that each iteration yields an improved value for the unknown parameters by reducing the criterion function.

There are many techniques that are classified as gradient methods; to examine all would require an enormous computational effort. This analysis will be restricted to the following methods, which are considered the most promising for computational efficiency:

- 1) Gauss-Newton^{55,56}
- 2) Conjugate Gradient⁵⁷⁻⁵⁹
- 3) Variable Metric⁶⁰⁻⁶²

References given for these methods pertain to their development as techniques for minimizing algebraic functions with explicit unknown parameters. In the next section, search directions for these methods are presented along with the advantages and disadvantages of the methods for distributive parameter identification. Also the methods of steepest descent¹⁰ and of Newton⁵⁵ are given to present comparisons with these three methods.

D. Gradient Search Directions

The method of steepest descent is the most widely used gradient method because of the ease of obtaining the search direction. It is chosen as the gradient of the criterion function, i.e.,

$$\underline{d}_i = - \frac{\partial Q(\underline{a}_i)}{\partial \underline{a}} , \quad (72)$$

where $\partial Q(\underline{a}_i)/\partial \underline{a}$ is an M-dimensional vector. However, the steepest-descent technique has a disadvantage when the solution of the identification problem is approached. The search directions given by Eq. 72 induce very small zigzag oscillations with each successive iteration, since only a short distance can be traveled in the steepest-descent direction before the descent property, Eq. 71 is violated. The ultimate number of iterations to reach a convergent solution is dependent upon the shape of the criterion function near the solution. The remaining gradient techniques to be discussed have convergence properties that are superior to those of the steepest-descent technique.

Newton's method seeks to improve the convergence in the vicinity of the solution by using information provided by the second derivative of the criterion function. The search direction is obtained by using a second-order Taylor-series expansion for the criterion function about its minimum to obtain the following search direction:

$$\underline{d}_i = - \left[\frac{\partial^2 Q(\underline{a}_i)}{\partial \underline{a} \partial \underline{a}^T} \right]^{-1} \frac{\partial Q(\underline{a}_i)}{\partial \underline{a}}, \quad (73)$$

where $\partial^2 Q(\underline{a}_i)/\partial \underline{a} \partial \underline{a}^T$ is the M by M-dimensional second-derivative matrix of the criterion function with respect to the unknown parameters. In the neighborhood of the solution, Newton's method is very efficient and convergence to the solution is very rapid. It is necessary to calculate ρ_i only for the first iteration, because the search direction given by Eq. 73 will satisfy the descent property with ρ_i equal to one as the solution is approached.

A difficulty exists in determining the second-derivative matrix and also in solving for its inverse. For the distributive-parameter system the evaluation of this matrix requires the solution of $\frac{1}{2}(M^2 + M)$ additional partial differential equations at each iteration when compared with the steepest-descent technique. Due to this computational difficulty, Newton's method has not been applied to the problem of distributive-parameter identification.

The remaining methods try to attain the convergence characteristics of Newton's method while eliminating some of its computational difficulties. Thus, the name quasi-Newton has been applied to these methods. The Gauss-Newton technique eliminates the necessity of calculating the second-derivative matrix and is based on a first-order Taylor-series expansion of the system variables to obtain the following search direction:

$$\underline{d}_i = \left[\frac{\partial u(\underline{a}_i)}{\partial \underline{a}} \frac{\partial u(\underline{a}_i)}{\partial \underline{a}}^T \right]^{-1} \frac{\partial u(\underline{a}_i)}{\partial \underline{a}}^T [\underline{y} - u(\underline{a}_i)], \quad (74)$$

where $\partial u(\underline{a}_i)/\partial \underline{a}$ is an N'RS by M-dimension matrix composed of the values at $\underline{a}_i$ of the derivative of the measured system variables (N' in number) with respect to the unknown parameters (M) at each of the measured points (RS) in the criterion function, Eq. 69. The N'RS-dimensional column vector $[\underline{y} - u(\underline{a}_i)]$ is the value of the difference between the measured values and the values of the system variables evaluated at $\underline{a}_i$. Methods of determining $\partial u(\underline{a}_i)/\partial \underline{a}$ are given in Sect. IV.E.

Convergence characteristics obtained from using the search direction given by Eq. 74 are superior to those of the steepest-descent technique and approach the characteristics of Newton's method. Similar to Newton's method, the value of ρ_i need only be calculated for the first few iterations in order to satisfy the descent property. The computational difficulty that exists with the Gauss-Newton method is the necessity of solving an M^{th} -order set of linear equations to evaluate the inverse of the matrix given in Eq. 74.

The remaining two methods, the conjugate gradient and the variable metric, do not require the solution of a set of linear equations in order to determine the search directions. They are based on the assumption that the criterion function behaves as a quadratic function in the neighborhood of the solution of the identification problem. Then the matrix of second derivatives of the criterion function can be considered to be essentially constant in this neighborhood. The search directions are then selected to be orthogonal or conjugate with respect to this second-derivative matrix. By denoting the second-derivative matrix as

$$\underline{G} = \left[\frac{\partial^2 Q(\underline{a})}{\partial \underline{a} \partial \underline{a}^T} \right], \quad (75)$$

the conjugacy requirement is given by

$$\underline{d}_i^T \underline{G} \underline{d}_j = 0 \quad \text{for } 0 \leq j \leq i-1. \quad (76)$$

When the successive search directions $\underline{d}_i$, $i = 1, 2, \dots$, satisfy Eq. 76, the convergence characteristics of the conjugate-gradient and variable-metric methods in the vicinity of the solution are similar to Newton's method.

The conjugate-gradient technique is the simpler of the two, and the search direction $\underline{d}_i$ is given by

$$\underline{d}_i = -\underline{g}_i + \frac{\underline{g}_i^T \underline{g}_i}{\underline{g}_{i-1}^T \underline{g}_{i-1}} \underline{d}_{i-1} \quad \text{for } i \geq 1, \quad (77)$$

where

$$\underline{g}_i = \frac{\partial Q(\underline{a}_i)}{\partial \underline{a}}. \quad (78)$$

For the initial search direction $\underline{d}_0$ the direction of steepest descent is chosen so that

$$\underline{d}_0 = -\underline{g}_0 \quad (79)$$

Search directions for the variable-metric technique are given by

$$\underline{d}_i = -\underline{H}_i \underline{g}_i \quad (80)$$

where

$$\underline{H}_i = \underline{H}_{i-1} + \frac{\Delta \underline{a}_{i-1} \Delta \underline{a}_{i-1}^T}{\Delta \underline{a}_{i-1}^T \Delta \underline{g}_{i-1}} - \frac{\underline{H}_{i-1} \Delta \underline{g}_{i-1} \Delta \underline{g}_{i-1}^T \underline{H}_{i-1}}{\Delta \underline{g}_{i-1}^T \underline{H}_{i-1} \Delta \underline{g}_{i-1}} \quad (81)$$

with

$$\Delta \underline{a}_{i-1} = \underline{a}_i - \underline{a}_{i-1} \quad (82)$$

and

$$\Delta \underline{g}_{i-1} = \underline{g}_i - \underline{g}_{i-1} . \quad (83)$$

The initial search direction is in the direction of steepest descent thus,

$$\underline{H}_0 = \underline{I} . \quad (84)$$

The $\underline{H}_i$ matrix is an M by M positive-definite matrix and is also equal to the inverse of the second-derivative matrix at the solution of the identification problem.

It would seem that these two methods would be the best to use, since they neither require the evaluation of the second-derivative matrix nor the solution of a set of linear equations. However, the necessary condition for generating search directions that satisfy Eq. 76 requires that the value of ρ_i be selected so that the criterion function is minimized in the direction $\underline{d}_i$, i.e.,

$$\frac{\partial Q(\underline{a}_i + \rho_i \underline{d}_i)}{\partial \rho_i} = 0 , \quad (85)$$

which implies that

$$\underline{g}_{i+1} \underline{d}_i = 0 . \quad (86)$$

Thus, the gradient of the criterion function at $\underline{a}_{i+1}$ is orthogonal to the previous search direction at the minimum of the criterion function along $\underline{d}_i$. The ultimate efficiency of these two methods depends upon the computational effort required in determining ρ_i to satisfy Eq. 86.

E. Gradient Evaluation

Each of the gradient methods relies upon evaluating the derivative of the system variables with respect to the unknown parameters. These values can then be used to calculate the gradient of the criterion function. The value of $\partial Q / \partial \underline{a}$ can be obtained by taking the partial derivative of the criterion function, Eq. 69, with respect to the unknown parameters, $\underline{a}$, to obtain the M^{th} -order vector:

$$\frac{\partial Q}{\partial \underline{a}} = \sum_{r=1}^R \sum_{s=1}^S -2 \frac{\partial \underline{u}(\underline{x}_r, t_s)^T}{\partial \underline{a}} [\underline{y}(\underline{x}_r, t_s) - \underline{u}(\underline{x}_r, t_s)] , \quad (87)$$

where $\partial \underline{u}(\underline{x}_r, t_s) / \partial \underline{a}$ is a N' by M -dimensional matrix and $[\underline{y}(\underline{x}_r, t_s) - \underline{u}(\underline{x}_r, t_s)]$ is a N' column vector. The value of the derivative of the system variables with respect to the unknown parameters can be evaluated by two methods.

One method of evaluating $\partial \underline{u}(\underline{x}_r, t_s) / \partial \underline{a}$ is to write a partial differential equation in $\partial \underline{u}(\underline{x}, t) / \partial \underline{a}$ by using the continuity relationship

$$\frac{\partial}{\partial \underline{a}} \left[\frac{\partial \underline{u}(\underline{x}, t)}{\partial t} \right] = \frac{\partial}{\partial t} \left[\frac{\partial \underline{u}(\underline{x}, t)}{\partial \underline{a}} \right] , \quad (88)$$

which yields the following set of MN' partial differential equations,

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{\partial \underline{u}}{\partial \underline{a}} \right) &= \frac{\partial \underline{F}}{\partial \underline{a}} + \frac{\partial \underline{F}}{\partial \underline{u}} \frac{\partial \underline{u}}{\partial \underline{a}} + \frac{\partial \underline{F}}{\partial \left(\frac{\partial \underline{u}}{\partial \underline{x}} \right)} \frac{\partial \left(\frac{\partial \underline{u}}{\partial \underline{x}} \right)}{\partial \underline{a}} \\ &+ \frac{\partial \underline{F}}{\partial \left(\frac{\partial^2 \underline{u}}{\partial \underline{x}^2} \right)} \frac{\partial \left(\frac{\partial^2 \underline{u}}{\partial \underline{x}^2} \right)}{\partial \underline{a}} . \end{aligned} \quad (89)$$

The coefficients of Eq. 89 can be obtained from the solution of the system equations given by Eq. 65. Equation 89 is often called the sensitivity equation since it relates a change in each of the unknown parameters to an effect on the system variables.

An alternative approach of evaluating the derivative of the system variables with respect to the unknown parameters is based on successive

solutions of Eq. 65 and then evaluation of the value of $\partial \underline{u}(x,t)/\partial \underline{a}$ by a "finite difference" approximation. A set of values for $\underline{u}(x,t)$ are obtained by perturbing each component of $\underline{a}$ individually by a small change $\delta \underline{a}$. Then the value of l^{th} component of the gradient of $\underline{u}(x,t)$ can be approximated by

$$\frac{\partial \underline{u}}{\partial a_l} \approx \frac{\underline{u}(\underline{a} + \delta a_l) - \underline{u}(\underline{a})}{\delta a_l} \quad \text{for } l = 1, 2, \dots, M, \quad (90)$$

where $\underline{u}(\underline{a} + \delta a_l)$ is the value of $\underline{u}(x,t)$ when the l^{th} component of $\underline{a}$ is perturbed by δa_l in the solution of Eq. 65. Errors in the calculation of $\partial \underline{u}(x,t)/\partial \underline{a}$ using Eq. 90 involve the proper selection of $\delta \underline{a}$. If $\delta \underline{a}$ is too small, inaccuracy results from the cancellation of significant figures in the subtraction of $\underline{u}(\underline{a})$ from $\underline{u}(\underline{a} + \delta a_l)$, whereas a choice of too large a value for $\delta \underline{a}$ will result in a poor value due to the truncation error in the difference equation.

Values for $\partial \underline{u}(x,t)/\partial \underline{a}$ obtained either by Eq. 90 or the solution of 89 are used to form the N'RS by M matrix $\partial \underline{u}(\underline{a})/\partial \underline{a}$ used in the Gauss-Newton method and also used in evaluating $\partial Q/\partial \underline{a}$ for the other gradient methods by using Eq. 87. Each technique of evaluating $\partial \underline{u}(x,t)/\partial \underline{a}$ involves the solution of M partial differential equations in addition to the solution of Eq. 65, which is used to evaluate the criterion function, Eq. 69. In general, Eq. 90 was used in this analysis. Errors occurring due to the selection of the $\delta \underline{a}$ value were minimized by normalizing the unknown parameters and using double-precision arithmetic on the computer. Sample calculations indicated a wide range of $\delta \underline{a}$ values could be used without affecting the values of $\partial \underline{u}(x,t)/\partial \underline{a}$. Both methods were used in evaluating $\partial \underline{u}(x,t)/\partial \underline{a}$ for the set of hyperbolic equations and yielded the same results. A slight increase in computational efficiency resulted when Eq. 90 was used.

F. Selection of ρ_i

According to the gradient method employed, the determination of ρ_i is based on satisfying various requirements. For the Gauss-Newton technique, ρ_i is selected so that successive iterations decrease the value of the criterion function. In satisfying this condition the value of ρ_i does not have to be determined uniquely, and a wide range of values can be chosen. In the case of the conjugate-gradient and variable-metric techniques, the value of ρ_i is used to minimize the criterion function in the search direction, $\underline{d}_i$, to provide the necessary condition of conjugate directions, Eq. 76, for the successive search directions. A problem exists in determining how accurate the value of ρ_i must be in order to insure the convergence characteristics of the conjugate-gradient and variable-metric techniques. Determination of ρ_i for the gradient methods is accomplished by a one-dimensional search technique.

For the Gauss-Newton method the following one-dimensional search technique proved to be the most successful for determining ρ_i . With the notation

$$Q[b] = Q(\underline{a}_i + \rho_i \underline{d}_i) \Big|_{\rho_i = b}, \quad (91)$$

the one-dimensional search technique is given as follows:

1. With the value of $Q[0]$ known from the previous iteration, evaluate $Q[1]$ and if $Q[1] < Q[0]$; then set $\rho_i = 1$.
2. If $Q[1] \geq Q[0]$, evaluate $Q[\frac{1}{2}]$ and use $\rho_i = \frac{1}{2}$ if $Q[\frac{1}{2}] < Q[0]$.
3. When $Q[\frac{1}{2}] \geq Q[0]$, a parabola is fit through the points $Q[0]$, $Q[1]$, and $Q[\frac{1}{2}]$, and a value for ρ_i is determined by the interpolation formula

$$\rho_i = \left| \frac{3/4Q[0] - \frac{1}{2}Q[\frac{1}{2}] + \frac{1}{4}Q[1]}{Q[0] - 2Q[\frac{1}{2}] + Q[1]} \right|. \quad (92)$$

This one-dimensional search technique will be denoted as Search A and is used exclusively for the Gauss-Newton method. It was obtained by combining several methods of one-dimensional search techniques that were given in the literature.⁸ Attempts to use this search technique for the conjugate-gradient and variable-metric methods failed except for the case of identifying one unknown parameter.

The one-dimensional search technique used for the conjugate-gradient and variable-metric techniques is based on determining ρ_i to a predefined accuracy μ^* and is given as follows:

1. Select a value of μ^* .
2. A second-order polynomial is used to obtain an initial estimate of ρ_i as

$$\rho_i = \frac{2Q[0]}{\underline{g}_i^T \underline{d}_i}, \quad (93)$$

where $\underline{d}_i$ depends upon the gradient method being employed.

3. The minimum value ρ_i is then bracketed by three values given by ζ_1 , ζ_2 , and ζ_3 , with $0 \leq \zeta_1 < \zeta_2 < \zeta_3$ and a set of corresponding Q values, Q_1 , Q_2 , and Q_3 with $Q_1 \geq Q_2$ and $Q_2 \leq Q_3$, which places the value of ρ_i between ζ_1 and ζ_3 . This value of ρ_i is determined by fitting a parabola through these ζ values and obtaining the interpolation formula

$$\rho_i = \frac{1}{2} \frac{(\zeta_2^2 - \zeta_3^2)Q_1 + (\zeta_3^2 - \zeta_1^2)Q_2 + (\zeta_1^2 - \zeta_2^2)Q_3}{(\zeta_2 - \zeta_3)Q_1 + (\zeta_3 - \zeta_1)Q_2 + (\zeta_1 - \zeta_2)Q_3}. \quad (94)$$

4. The search range of ζ values is reduced, and the process continues until successive values of ρ_i given by Eq. 94 differ by less than μ^* .

This search technique, known as Search B, is based on a modification of a method suggested by Bard¹³ and has yielded good results. As the required accuracy of the ρ_i value is increased, the required computations increased, and studies were made to determine the best value to shorten the computation time. Results showed that a value of 0.01 for μ^* usually determined ρ_i accurately to insure convergence of the conjugate-gradient and variable-metric techniques.

Before performing the one-dimensional search, several tests are made to decrease the computational effort and prevent erroneous search directions. If the gradient of the criterion function is zero, the search is terminated, since the basis for all of the methods is that the gradient is zero at the minimum. After the search direction $\underline{d}_i$ is determined, a test is made to insure that the criterion function will decrease along that direction. This is accomplished by requiring that

$$\underline{d}_i^T \underline{g}_i < 0 . \quad (95)$$

If Eq. 95 is not satisfied, the search direction $\underline{d}_i$ is changed to the direction of steepest descent for the conjugate-gradient and variable-metric techniques.

To improve the convergence characteristic for the conjugate-gradient and variable-metric techniques, the search directions were periodically modified by discarding the previous search values and using the steepest-descent direction as the new search direction. This modification was made for every $(M + 1)$ iteration, where M is the number of unknown parameters, to retain the possibility of the M iterations convergence characteristics of these two methods for quadratic functions (see Appendix C). For the examples in this study the use of steepest descent for every $(M + 1)$ iteration usually improved the convergence characteristics of the conjugate-gradient and variable-metric techniques.

G. Convergence Criterion

With the use of iterative techniques a problem exists in determining when the sequence of $\underline{a}_i$ values, $i = 1, 2, \dots$, have converged to the solution of the identification problems. The values of $\underline{a}_i$ for each iteration are determined by the minimization of $Q(\underline{a}_i)$, and a solution occurs when the values of $Q(\underline{a}_i)$, $i = 1, 2, \dots$, converge to the global minimum of Q . Although none of the known iterative methods, including the gradient techniques, can guarantee to locate the global minimum rather than a local minimum, a reasonable assumption is made that the Q function is either globally concave or only one minimum of Q exists in the region of the initial approximation of the $\underline{a}$ values. Thus, a good initial value for $\underline{a}$ is sometimes a necessity to obtain the correct solution.

The selection of a convergence criterion can be based on the assumption that the direction vector $\underline{d}_i$ is selected to be one of the best available. Then it is possible to consider a convergence criterion based on the successive values of $\underline{a}_i$. When the difference between these successive values is less than some prescribed value, convergence is said to have occurred. The convergence criterion to be used in this analysis is given by

$$\sum_{l=1}^M \left| \frac{a_{l,i+1} - a_{l,i}}{a_{l,i+1}} \right| \leq \mu . \quad (96)$$

A similar choice could have been made with successive values of $Q(\underline{a}_i)$, but in general the convergent value would be the same as that obtained by using Eq. 96 provided the μ value was changed for use with criteria using $Q(\underline{a}_i)$ values. Any difference between using Eq. 96 and successive $Q(\underline{a}_i)$ values would occur only if the shape function was very skewed near the minimum value. A further check on the results obtained can be made by checking the value of the criterion function to see how well the values of the measured system variables agree with the data that were originally supplied.

H. Summary and Algorithm for Distributive-parameter Identification

In Table IX the formulation of the search directions are given for the steepest descent, Newton's, and three quasi-Newton techniques. To solve the problem of distributive-parameter identification the following algorithm is employed:

1. Choose an initial value for the unknown parameter, $\underline{a}_0$ for $\underline{a}_i$.
2. With the values of $\underline{a}_i$ solve Eq. 65 for the system variables.
3. Evaluate criterion function, Eq. 69.
4. Solve for the gradient of the system variables with respect to $\underline{a}$, using either Eq. 89 or 90, and then evaluate the gradient of the criterion function, Eq. 87.
5. Evaluate the search direction, $\underline{d}_i$, for the gradient technique being employed. This requires the solution of a set of M linear equations for the Gauss-Newton method.
6. Determine the appropriate value of ρ_i depending upon the gradient method being used.
7. Determine the value of $\underline{a}_{i+1}$ using Eq. 70 and then test for convergence using Eq. 96. If Eq. 96 is satisfied, the process is stopped.
8. If Eq. 96 is not satisfied, repeat steps 2 through 8 using the values of $\underline{a}_{i+1}$ for $\underline{a}_i$.

In Ch. V this algorithm has been used with each of the quasi-Newton gradient techniques for three representative distributive-parameter systems.

TABLE IX. Gradient Search Direction

Method	$\underline{d}_i$
Steepest Descent	$-\underline{g}_i$
Newton	$-\underline{G}^{-1}$
Gauss-Newton	$-\left[\begin{array}{cc} \frac{\partial u^T}{\partial \underline{a}} & \frac{\partial u}{\partial \underline{a}} \end{array} \right]^{-1} \underline{g}_i$
Conjugate Gradient	$-\underline{g}_i + \frac{\underline{g}_i^T \underline{g}_i}{\underline{g}_{i-1}^T \underline{g}_{i-1}} \underline{d}_{i-1}$
Variable Metric	$-\underline{H}_i \underline{g}_i$
	with
	$\underline{H}_i = \underline{H}_{i-1} + \frac{\Delta \underline{a}_{i-1} \Delta \underline{a}_{i-1}^T}{\Delta \underline{a}_{i-1}^T \Delta \underline{g}_{i-1}}$
	$- \frac{\underline{H}_{i-1} \Delta \underline{g}_{i-1} \Delta \underline{g}_{i-1}^T \underline{H}_{i-1}}{\Delta \underline{g}_{i-1}^T \underline{H}_{i-1} \Delta \underline{g}_{i-1}}$

V. NUMERICAL RESULTS OF DISTRIBUTIVE PARAMETER IDENTIFICATION

A. Introduction

In this chapter, the previously developed gradient methods are applied to several models of physical processes whose behavior can be described by partial differential equations. Two of the models chosen are linear, and describe phenomena encountered in heat-transfer and fluid-flow problems. The third model is a space- and time-dependent analysis of a nuclear reactor core which is a nonlinear model comprised of neutron-diffusion and thermohydraulic equations. The partial differential equations are solved by making use of finite-difference approximations for the partial derivatives. To reduce the computational difficulties the analysis has been limited to a single spatial dimension for all models.

Distributive-parameter systems that are analyzed in this chapter were selected to illustrate the importance of parameter identification in a nuclear reactor system. The first model consists of a single parabolic partial differential equation which illustrates the dynamic analysis of heat-transfer and fluid-flow processes. These processes are often the limiting factors in the safe and efficient operation of the nuclear reactor. Parameters in this parabolic equation are generally obtained from the analysis of experimental results and the identification techniques can be used to analyze the data and assist in obtaining more reliable values for these parameters. Often there exists some uncertainty in the applicability of a model to a particular physical process. For ease of analysis the engineer tries to use the simplest model that will approximate the physical process. Parameter identification can be used in model development to yield the desired accuracy and complexity. This is illustrated for the parabolic equation by progressively adding terms to the equation and determining increasing numbers of unknown parameters.

Another application of parameter-identification techniques is in the determination of changes that occur in an operating system over a period of time. This is illustrated by the second example of a counter-current, double-pipe heat exchanger. During the operation of the heat exchanger, deposition of foreign materials on the walls of the heat exchanger may change its heat-transfer characteristics. By using the parameter-identification techniques the changes in heat-transfer coefficients are identified; this permits preventive maintenance to return the plant to normal operations. The heat-exchanger model consists of two coupled hyperbolic partial differential equations. This example and the previous one based on a parabolic equation illustrate the application of identification techniques to individual processes or components in a nuclear power plant. The next example shows the application of parameter identification to the response of a nuclear reactor which includes the applicable heat-transfer and fluid-flow processes.

The nuclear reactor model developed in Ch. III is extended to include time-dependent changes in the power level. This nonlinear, space-dependent model is analyzed for increasing and decreasing power levels caused by reactivity insertions in the core. Transient conditions will be caused by step and ramp changes in the nuclear cross sections, and the magnitude of

these changes will be identified. These transient conditions illustrate power-level changes that are made in the reactor by the insertion or removal of control rods.

B. Parabolic Partial Differential Equations

Each of the examples of parameter identification using a single parabolic partial differential equation are a simplified form of the following equations:

$$\frac{\partial u(x,t)}{\partial t} = a_1 \frac{\partial^2 u(x,t)}{\partial x^2} + a_2 \frac{\partial u(x,t)}{\partial x} + a_3 u(x,t) \quad (97)$$

$$\text{for } 0 < x < L; \quad t > 0$$

with the constraint of $a_1 > 0$. The boundary and initial conditions were chosen as

$$u(0,t) = 0; \quad u(L,t) = 0; \quad u(x,0) = \sin x$$

for a length $L = \pi$. Equation 97 is solved numerically by an implicit finite-difference formulation to insure numerical stability for any arbitrary choice of parameter values and of space and time mesh spacings. Specifically, the Crank-Nicolson⁶³ implicit difference formulas were employed to reduce the partial differential equation to a set of algebraic equations. By using Δx and Δt to represent the space and time mesh spacings, respectively, and denoting the value of $u(j\Delta x, k\Delta t)$ as $u_{j,k}$, Eq. 97 is written in the following finite-difference form:

$$\begin{aligned} u_{j+1,k+1} \left[-1 - \frac{a_2 \Delta x}{2a_1} \right] + u_{j,k+1} \left[2 + \frac{2\Delta x^2}{a_1 \Delta t} - \frac{a_3 \Delta x^2}{a_1} \right] \\ + u_{j-1,k+1} \left[-1 + \frac{a_2 \Delta x}{2a_1} \right] = u_{j+1,k} \left[1 + \frac{a_2 \Delta x}{2a_1} \right] \\ + u_{j,k} \left[-2 + \frac{2\Delta x^2}{a_1 \Delta t} + \frac{a_3 \Delta x^2}{a_1} \right] + u_{j-1,k} \left[1 - \frac{a_2 \Delta x}{2a_1} \right]. \quad (98) \end{aligned}$$

Equation 98 is valid for $1 \leq j \leq J-1$ and $k \geq 1$, with the known spatial boundary conditions designated at $j = 0$ and $j = J$ and known initial conditions given for $k = 0$. By using Eq. 98, a set of $(J-1)$ equations are written for the unknown dependent variable at time step $k+1$ and spatial mesh values of $j = 1, 2, \dots, J-1$. This set of equations produce a $(J-1)$ by $(J-1)$ tridiagonal matrix equation of the form

$$\underline{B} \underline{w} = \underline{s}, \quad (99)$$

where the diagonal elements of $\underline{B}$ are given by $[2 + (2\Delta x^2/a_1\Delta t) - (a_3\Delta x^2/a_1)]$, the lower off-diagonal elements of $\underline{B}$ are $[-1 + (a_2\Delta x/2a_1)]$, and the upper off-diagonal elements are $[-1 - (a_2\Delta x/2a_1)]$. The $(J-1)$ -dimensional vector $\underline{w}$ is composed of the values of $u_{j,k+1}$, $j = 1, 2, \dots, J-1$, and the elements of $\underline{s}$ are given by

$$\begin{aligned} s_j = & u_{j+1,k} \left[1 + \frac{a_2\Delta x}{2a_1} \right] + u_{j-1,k} \left[1 - \frac{a_2\Delta x}{2a_1} \right] \\ & + u_{j,k} \left[-2 + \frac{2\Delta x^2}{a_1\Delta t} + \frac{a_3\Delta x^2}{a_1} \right]; \end{aligned} \quad (100)$$

$$j = 1, 2, \dots, J-1.$$

Equation 99 is solved by use of a Gaussian elimination technique for a tridiagonal matrix.^{64,65}

Although the Crank-Nicolson technique is unconditionally stable for any values of Δx and Δt , these values must be chosen so that the numerical solution will approximate the analytical solution of the partial differential equation. In the examples presented in this section, values of $\Delta x = \pi/20$ and $\Delta t = 0.005$ were used, and the resulting numerical solution was in error by approximately 0.01% from the known analytic solution⁶⁶ of Eq. 97.

In applying the parameter-identification techniques presented in Ch. IV, a problem exists with the constraint of $a_1 > 0$, since each of the gradient techniques is based upon unconstrained minimization, for which any values of the unknown parameters are allowed. To insure that a_1 remains greater than zero for each iteration, the value of ρ_i as determined by the methods discussed in Sect. IV.F is restricted to a certain range of values. Since the updated values for the unknown parameters depend upon the selection of ρ_i , the convergence of the gradient methods may be impaired due to the constraint on a_1 . For the Gauss-Newton technique, the effect is minimal, since the value of ρ_i is not required to be uniquely determined. However, for the conjugate-gradient and variable-metric techniques the selection of ρ_i must also satisfy the conjugacy requirements, Eq. 76, for successive search directions, and it may be impossible to satisfy both Eq. 76 and the constraint on a_1 . Therefore, if the search direction is selected only on satisfying the constraint $a_1 > 0$, the values of successive search directions may be erroneous. To overcome this problem, several tests are made before the ρ_i value is selected. These tests were outlined in Sect. IV.F and result in the selection of a new search direction based upon the direction of steepest descent.

The success of the iterative identification procedure is determined when the parameter values satisfy the convergence criterion, Eq. 96, with the value of μ selected as 10^{-4} . The choice for μ was based upon an analysis using several values of μ , and comparing the variations of the parameter

and criterion-function values for the different μ values. Using values of μ less than 10^{-4} resulted in only a slight increase in the accuracy of the solutions for most of the example problems, whereas the number of iterations increased significantly. Increasing the μ value from 10^{-4} resulted in a significant decrease in the accuracy of the solution.

Calculation of the derivatives of the system variables with respect to the unknown parameters was accomplished by using the finite-difference method, Eq. 90. The value for δa was chosen to be 10^{-8} for all of the calculations, since there was no perceptible difference in these gradient values as compared with the values obtained from the solution of the sensitivity equations, given by Eq. 89. The number of partial differential equations that must be solved to obtain the final parameter values is used as for comparison of the efficiencies of each of the gradient techniques. This is a valid approach since the computational time for other calculations are negligible when compared with the time required for solutions of the partial differential equation.

1. Identification of One Parameter.

By setting a_2 and a_3 in Eq. 97 equal to zero, the simplest parabolic partial differential equation is obtained:

$$\frac{\partial u(x,t)}{\partial t} = a_1 \frac{\partial^2 u(x,t)}{\partial x^2} . \quad (101)$$

Identification of one parameter presents an unusual case since it is possible to obtain the solution by using only a one-dimensional search technique. This is accomplished by evaluating the gradient, using the initial parameter estimate, and then using Search B as outlined in Sect. IV.F for the one-dimensional search. The tolerance μ^* for Search B is selected as the desired accuracy of the identification, which is 10^{-4} in this analysis.

The example problem for the case of one unknown parameter was selected as $a_1 = 0.9$. Ten values of $u(x,t)$ at the points $\pi/4$ and $\pi/2$ for time steps of 0.2 sec were used as the system measurements. Results were obtained using initial estimates of 0.5 and 4.0 for a_1 . With only Search B used, the value of a_1 was identified as 0.90001, with a corresponding criterion function value of 0.5714×10^{-10} . This result required seven solutions of Eq. 101 to obtain the desired accuracy.

The Gauss-Newton technique was then applied to this example with Search A used to determine ρ_i . In four iterations with ten solutions of Eq. 101, the same value for a_1 as given above was obtained. The conjugate-gradient and variable-metric techniques were used for this problem by making a slight modification in Search A. This change was necessary since the search directions given by these two techniques are not normalized, and thus the initial ρ_i value is given by Eq. 93 instead of the 1.0 used with the Gauss-Newton method. Both techniques converged to the above solution in four iterations, with thirteen solutions of Eq. 101 required.

The most efficient method of determining a single unknown parameter is the use of Search B with μ^* the desired accuracy of identification.

2. Identification of Two Parameters.

The first-order derivative of $u(x,t)$ with respect to x is added to Eq. 101 to illustrate the identification of two parameters, with the model equation given by

$$\frac{\partial u(x,t)}{\partial t} = a_1 \frac{\partial^2 u(x,t)}{\partial x^2} + a_2 \frac{\partial u(x,t)}{\partial x} . \quad (102)$$

The Gauss-Newton technique with Search A and the conjugate-gradient and variable-metric methods using Search B with $\mu^* = 10^{-2}$ are used exclusively in the identification of a_1 and a_2 .

Values of a_1 and a_2 were selected as 1.0 and 0.1, respectively, while measurements were employed for three spatial positions, $\pi/4$, $\pi/2$, and $3\pi/4$, and for five time steps of 0.2 sec. When the initial estimates were made in the proximity of the values $a_1 = 0.9$ and $a_2 = 0.2$, each of the gradient techniques required four iterations to obtain the following solution:

$$a_1 = 1.0; a_2 = 0.099996; Q = 0.1302 \times 10^{-9} .$$

However, the Gauss-Newton method required only fifteen solutions of Eq. 102 to obtain this result, whereas the conjugate-gradient and variable-metric methods required twenty-three and thirty-one solutions, respectively. When initial estimates of a_1 and a_2 were less accurate ($a_1 = 0.5$ and $a_2 = -0.3$), there was a greater disparity between the efficiencies of the gradient techniques. Results of this analysis are given in Table X. The modified conjugate-gradient and variable-metric methods refer to the recycling of the search directions to the direction of steepest descent after every third iteration. With this recycling to eliminate any erroneous search directions, the number of solutions of Eq. 102 required to obtain the solution was reduced. There is also a very slight decrease in the accuracy of the identification when the conjugate-gradient method was used.

A second set of a_1 and a_2 values ($a_1 = 1.0$ and $a_2 = -1.0$) were used to study the effects of varying initial parameter estimates upon the rate of convergence and accuracy of the solution. When initial estimates were close to the true values (25% error), each of the gradient methods yielded the same result of 1.0 and -1.0 for a_1 and a_2 , respectively, with $Q = 0.1540 \times 10^{-9}$. The number of iterations and equation solutions required for this solution were similar to the values given in Table X for the previous case. When initial estimates were less accurate (500% error), the Gauss-Newton technique yielded the same results and usually required only one additional iteration. The other gradient techniques usually required several more iterations and also exhibited a slightly less accurate result for some sets of initial parameter values. These derivations were so negligible that the resulting parameter values were still very accurate.

TABLE X. Identification of Two Parameters in a Parabolic Equation

Method ^a	GN	CG	CGM	VM	VMM
One-dimensional Search ^b Technique	A	B, 10 ⁻²	B, 10 ⁻²	B, 10 ⁻²	B, 10 ⁻²
a ₁	1.0	1.0	1.0	1.0	1.0
a ₂ (10)	0.99996	1.0001	0.99998	0.99996	0.99996
Q(10 ⁹)	0.1302	0.1429	0.1307	0.1302	0.1302
Number of Iterations	5	9	7	6	6
Number of Solutions of PDE ^c	18	67	59	47	45

^aGN - Gauss-Newton

CG - Conjugate Gradient

CGM - Modified Conjugate Gradient

VM - Variable Metric

VMM - Modified Variable Metric

^bA - Search AB, 10⁻² - Search B
with $\mu^* = 10^{-2}$ ^cPDE - Partial Differential
Equations

In summary, the Gauss-Newton technique was the most accurate and efficient of the techniques for the identification of two parameters.

3. Identification of Three Parameters.

The three unknown parameters in Eq. 97 are now identified with values for a_1 , a_2 , and a_3 being 1.0, -2.0, and -1.0, respectively. Fifteen measured values were again used, and Table XI gives the results of the identification when initial parameter estimates of 0.9, -1.9, and -0.9 were made.

The steepest-descent technique was used to provide a comparison for the other methods, and it was the only technique that failed to reach a convergent solution for this example. An important result shown in Table XI is the significantly less accurate values obtained with both forms of the variable-metric technique. Although the modified version of the variable-metric technique did reduce the error as depicted by the criterion function by two orders of magnitude, the resulting solution is still significantly less accurate than the other methods.

The choice of μ^* in Search B for the conjugate-gradient and variable-metric method influences not only the rate of convergence, but also the accuracy of the solution. In Table XII the results of varying μ^* for the conjugate-gradient method are shown for the initial estimates of 0.9, -1.9, and -0.9 for the unknown parameters. Although the results of Table XII clearly indicate the best value of $\mu^* = 10^{-2}$ for this problem,

TABLE XI. Identification of Three Parameters in a Parabolic Equation

Method	SD ^a	GN	CG	CGM	VM	VMM
One-dimensional Search Technique	B,10 ⁻²	A	B,10 ⁻²	B,10 ⁻²	B,10 ⁻²	B,10 ⁻²
a ₁	0.98385	0.99999	1.0001	0.99997	0.98124	0.99815
a ₂	-1.9864	-2.0	-2.0	-2.0	-1.9841	-1.9984
a ₃	-1.0194	-1.0	-0.99992	-1.0	-1.0229	-1.0023
Q(10 ⁹)	107	0.1266	0.1463	0.1298	1468	14.26
Number of Interactions	20 ^b	4	7	9	7	18
Number of PDE Solutions	185	20	55	75	70	141

^aSD - Steepest Descent^bSearch terminated after 20 iterationsTABLE XII. Effect of μ^* Value on Conjugate-Gradient Technique

μ value	10 ⁻¹	10 ⁻²	10 ⁻³	10 ⁻⁴
a ₁	1.0002	1.0001	0.99998	0.99998
a ₂	-2.0	-2.0	-2.0	-2.0
a ₃	-0.99987	0.99992	-1.0	-1.0
Q(10 ⁹)	0.1461	0.1463	0.1274	0.1274
Number of Interactions	12	7	7	7
Number of PDE Solutions	92	55	73	84

it should be emphasized that this value may not be the best for all further calculations with the conjugate-gradient method. The effect of various μ^* values for the variable-metric technique is easily illustrated by examining the results presented in Table XI. When μ^* was equal to 10⁻² very poor results were obtained; however, when the value of μ^* was decreased, the following results were obtained for the same problem.

$$\begin{aligned}
 a_1 &= 0.99988 & a_2 &= -2.0 \\
 a_3 &= -1.0 & Q &= 0.1273 \times 10^{-9}
 \end{aligned}$$

which were obtained in fifteen iterations with 136 solutions of Eq. 97.

Thus, it has been shown that the accuracy and efficiency of the conjugate-gradient and variable-metric technique can be significantly changed by use of a different μ^* value for the one-dimensional search.

Initial estimates of the parameters were again varied to determine their effect upon the efficiency and accuracy of the gradient techniques. Results that were obtained were similar to the two-parameter case, with the Gauss-Newton technique being superior in efficiency and accuracy when compared with the other gradient techniques.

C. Hyperbolic Partial Differential Equations

Under certain assumptions the dynamic behavior of a counter-current heat exchanger is described by the following coupled hyperbolic equations:

$$\frac{\partial u(x,t)}{\partial t} = -b_1 \frac{\partial u(x,t)}{\partial x} - a_1[u(x,t) - v(x,t)] ; \quad (103)$$

$$\frac{\partial v(x,t)}{\partial t} = b_2 \frac{\partial v(x,t)}{\partial x} + a_2[u(x,t) - v(x,t)] . \quad (104)$$

The dependent variables, $u(x,t)$ and $v(x,t)$, are the temperature values of the fluids, b_1 and b_2 their velocities. Parameters a_1 and a_2 contain the heat-transfer coefficients and will be identified in this analysis. The dynamic analysis will be made for a step change in the temperature, $u(x,t)$, at the inlet of the heat exchanger.

Equations 103 and 104 are solved numerically by an implicit centered finite-difference technique.⁶⁷ The finite-difference equations form a set of algebraic equations which are in the form of a bi-tridiagonal matrix at each time step. With Δx and Δt representing space and time mesh spacings, respectively, and the values of $u(j\Delta x, k\Delta t)$ denoted by $u_{j,k}$, those of $v(j\Delta x, k\Delta t)$ by $v_{j,k}$, Eqs. 103 and 104 are written in the following finite-difference form:

$$\begin{aligned} \left[-\frac{b_1}{\Delta x} + \frac{a_1}{2} + \frac{1}{\Delta t} \right] u_{j-1,k+1} + \left[\frac{b_1}{\Delta x} + \frac{a_1}{2} + \frac{1}{\Delta t} \right] u_{j,k+1} - \frac{a_1}{2} v_{j,k+1} \\ - \frac{a_1}{2} v_{j+1,k+1} = \left[\frac{b_1}{\Delta x} - \frac{a_1}{2} + \frac{1}{\Delta t} \right] u_{j-1,k} + \left[-\frac{b_1}{\Delta x} - \frac{a_1}{2} + \frac{1}{\Delta t} \right] u_{j,k} \\ + \frac{a_1}{2} v_{j+1,k} + \frac{a_1}{2} v_{j,k} ; \end{aligned} \quad (105)$$

$$\begin{aligned}
& \frac{a_2}{2} u_{j-1,k+1} + \frac{a_2}{2} u_{j,k+1} + \left[-\frac{b_2}{\Delta x} - \frac{a_2}{2} - \frac{1}{\Delta t} \right] v_{j,k+1} \\
& + \left[\frac{b_2}{\Delta x} - \frac{a_2}{2} - \frac{1}{\Delta t} \right] v_{j+1,k+1} = \left[\frac{b_2}{\Delta x} + \frac{a_2}{2} - \frac{1}{\Delta t} \right] v_{j,k} \\
& + \left[-\frac{b_2}{\Delta x} + \frac{a_2}{2} - \frac{1}{\Delta t} \right] v_{j+1,k} - \frac{a_2}{2} u_{j,k} - \frac{a_2}{2} u_{j-1,k} .
\end{aligned} \tag{106}$$

Equations 105 and 106 are valid for $1 < j < J$ with slight modifications at the boundary values of $j = 1$ and $j = J$ to account for the known boundary conditions. These finite difference equations are solved by means of an algorithm for bi-tridiagonal matrices.⁶⁵ An analytic solution for Eqs. 103 and 104 is available, and the results obtained using the centered difference technique have been compared favorably with the analytic solution.⁶⁸ For the examples to be presented in this analysis the numerical results were obtained with $\Delta x = L/20$ and $\Delta t = \Delta x/b_1$. The choice of $\Delta t = \Delta x/b_1$ minimizes the truncation error for the analysis of the problem of a step change in the temperature, $u(x,t)$, at $x = 0$. The only problem encountered with using the centered difference formulation is a slight oscillation in the neighborhood of the step change in $u(x,t)$, but this oscillation is present only as the perturbation passes through the heat exchanger.

Parameters a_1 and a_2 are positive values, and the determination of ρ_i is restricted to insure that a_1 and a_2 are positive for each iteration. The Gauss-Newton technique uses Search A to determine ρ_i while Search B with $\mu^* = 10^{-2}$ was used for the other techniques. The value of μ in the convergence criterion was again selected as 10^{-4} . Two methods were employed to determine the gradient of the system variables with respect to a_1 and a_2 . Results from the solution of the sensitivity equation were identical to the results obtained by using the finite-difference approach. Measurement values were obtained at the outlet of both the primary and secondary sides of the heat exchanger. Three forms of the criterion function were utilized in this analysis: the first form used only $u(L,t)$ measurements, the second used $v(0,t)$ values, while the third combined both sets of measurements.

The following example illustrates the identification of a_1 and a_2 for a heat exchanger with a normalized length of 1 ft. Zero initial and boundary conditions are set for $u(x,t)$ and $v(x,t)$ with measurement values for 0.5-sec intervals. Five measurement values were chosen, corresponding to the parameter values

$$\begin{array}{ll}
a_1 = 0.05 \text{ sec}^{-1} & b_1 = 1.0 \text{ ft/sec} \\
a_2 = 0.05 \text{ sec} & b_2 = 1.0 \text{ ft/sec}
\end{array}$$

for a 1.0°F step change at $u(0,0)$. Initial estimates for a_1 and a_2 were 0.3 and 0.2, and the mesh spacings were chosen as $\Delta x = 0.05$ ft and

$\Delta t = 0.05$ sec. Results of this analysis for each gradient technique and each form of the criterion function are given in Tables XIII through XV.

TABLE XIII. Parameter Identification Based upon $u(L,t)$ Measurements

Method	GN	CG	CGM	VM	VMM
$a_1(10)$	0.49993	0.50007	0.49993	0.4993	0.49993
$a_2(10)$	0.49761	0.50353	0.49760	0.49760	0.49767
$Q(10^{10})$	0.2829	1.957	0.2829	0.2829	0.2831
Number of Iterations	7	6	8	12	11
Number of PDE Solutions	24	48	69	91	79

TABLE XIV. Parameter Identification Based upon $v(0,t)$ Measurements

Method	GN	CG	CGM	VM	VMM
$a_1(10)$	0.49845	0.56319	0.50062	0.49922	0.49883
$a_2(10)$	0.49999	0.50107	0.50002	0.50000	0.49999
$Q(10^{10})$	0.1756	40.739	0.2032	0.1790	0.1759
Number of Iterations	7	7	9	19	12
Number of PDE Solutions	24	58	76	146	86

TABLE XV. Parameter Identification Based upon $u(L,t)$ and $v(0,t)$ Measurements

Method	GN	CG	CGM	VM	VMM
$a_1(10)$	0.49999	0.49999	0.49999	0.49999	0.49999
$a_2(10)$	0.50001	0.50001	0.50001	0.50001	0.50002
$Q(10^{10})$	0.7454	0.7454	0.7454	0.7453	0.7737
Number of Iterations	5	6	6	8	7
Number of PDE Solutions	18	33	33	49	43

Aside from the obvious superiority of the Gauss-Newton technique, several other results may be noted. The conjugate-gradient methods were substantially more efficient than the variable-metric methods but exhibited convergence to poorer results in certain cases. Use of measurements of $u(x,t)$ and $v(x,t)$ yielded the best results obtained. Identification of a_1 was more accurate when $u(L,t)$ measurements were used, and a_2 was more accurately determined when $v(0,t)$ measurements were used. This should be expected since a_1 is directly related to the $u(x,t)$ equation while a_2 is directly related to the $v(x,t)$ equation.

Three other examples of heat exchangers were analyzed with similar results. Parameter values for these examples were obtained in the literature⁶⁸⁻⁷⁰ to correspond to heat-exchanger models with various types of fluids and dimensions. Results that were obtained for all models indicated that the Gauss-Newton technique was the most efficient method for parameter-identification systems modeled by hyperbolic equations.

D. Space-Time-dependent Nuclear Reactor Model

The space-time-dependent nuclear reactor model for an LMFBR is based on the space-dependent model developed in Ch. III. This analysis is made for a model with a single neutron-energy group and uses a "prompt jump" or "zero neutron lifetime" model⁷¹ to reduce the computational problems. This model is sufficiently accurate for the transient analysis of the reactor when small reactivity changes are made in the reactor. Equations describing this model are

$$\begin{aligned}
 0 &= \frac{\partial}{\partial x} D(x) \frac{\partial}{\partial x} \phi(x,t) + [\Sigma_p(x) - \Sigma_a(x)] \phi(x,t) \\
 &\times [1 + a_f' \Delta \bar{T}_f(x,t) + a_c' \Delta T_c(x,t)] + \lambda C(x,t) \\
 &+ (1 - \beta) v \Sigma_f(x) \phi(x,t) [1 + a_f \Delta T_f(x,t) + a_c \Delta T_c(x,t)] ; \quad (107)
 \end{aligned}$$

$$\frac{\partial C(x,t)}{\partial t} = \beta v \Sigma_f(x) \phi(x,t) [1.0 + a_f \Delta \bar{T}_f(x,t) + a_c \Delta T_c(x,t)] - \lambda C(x,t) ; \quad (108)$$

$$\begin{aligned}
 \frac{\partial \bar{T}_f(x,t)}{\partial t} &= k_1 [T_c(x,t) - \bar{T}_f(x,t)] + k_2 \Sigma_f(x) \phi(x,t) \\
 &\times [1 + a_f \Delta \bar{T}_f(x,t) + a_c \Delta T_c(x,t)] ; \quad (109)
 \end{aligned}$$

$$\frac{1}{v_c} \frac{\partial T_c(x,t)}{\partial t} = - \frac{\partial T_c(x,t)}{\partial x} + k_3 [\bar{T}_f(x,t) - T_c(x,t)] - k_4 \Sigma_f(x) \phi(x,t) [1 + a_f \Delta \bar{T}_f(x,t) + a_c \Delta T_c(x,t)] ; \quad (110)$$

$$\Delta \bar{T}_f(x,t) = \bar{T}_f(x,t) - \bar{T}_f(0,0) ; \quad (111)$$

$$\Delta T_c(x,t) = T_c(x,t) - T_c(0,0) , \quad (112)$$

where

$\phi(x,t)$	- neutron flux
$C(x,t)$	- concentration of delayed-neutron precursors
$\bar{T}_f(x,t)$	- average fuel temperature
$\bar{T}_c(x,t)$	- coolant temperature
$D(x)$	- diffusion coefficient
$\Sigma_p(x)$	- poison control to maintain initial criticality
$\Sigma_a(x)$	- absorption cross section
$\Sigma_f(x)$	- fission cross section
v	- average number of neutrons per fission
λ	- delayed-neutron decay constant
β	- delayed-neutron fraction
a_f, a_c, a'_f, a'_c	- temperature-feedback coefficients
k_1, k_2, k_3, k_4	- thermal hydraulic constants
v_c	- coolant velocity

Boundary conditions for this set of equations are given by zero values for neutron flux at the spatial boundaries and known temperature values at the inlet ($x = 0$). Initial conditions are based on a critical reactor by determining $\Sigma(x)$. Values of neutron cross sections are given in Table I, and thermal^Phydraulic constants are available from Appendix A. The value of β is equal to 2.96×10^{-3} , that of $\lambda = 0.1$. Temperature-feedback coefficients are the same as those used in Ch. III:

$$\begin{aligned} a_f &= -0.4 \times 10^{-5}/^{\circ}\text{C} ; & a'_f &= +0.4 \times 10^{-6}/^{\circ}\text{C} ; \\ a_c &= -0.2 \times 10^{-4}/^{\circ}\text{C} ; & a'_c &= -0.4 \times 10^{-5}/^{\circ}\text{C} . \end{aligned}$$

From steady-state conditions a step and ramp change in reactivity is made to produce a positive or negative transient condition. This reactivity change is modeled by a time- and space-dependent change in the absorption cross section of the reactor, given by

$$\delta \Sigma_a(x,t) = (a_1 + a_2 t) \Sigma'(x), \quad (113)$$

where $\Sigma'(x)$ is a region-dependent cross-section value; a_1 and a_2 are the unknown parameters. Equation 113 is inserted into Eq. 107 to yield

$$\begin{aligned} 0 = & \frac{\partial}{\partial x} D(x) \frac{\partial}{\partial x} \phi(x,t) + [\Sigma_p(x) - \Sigma_a(x) \\ & + (a_1 + a_2 t) \Sigma'(x)] \phi(x,t) [1 + a_f' \Delta \bar{T}_f'(x,t) \\ & + a_c' T_c(x,t)] + \lambda C(x,t) + (1 - \beta) v \Sigma_f(x) \\ & \times [1 + a_f' \Delta \bar{T}_f'(x,t) + a_c' \Delta T_c(x,t)] . \end{aligned} \quad (114)$$

To obtain the solution of the set of differential equations, the partial derivatives with respect to the spatial variable are replaced by a finite-difference approximation to obtain a set of ordinary differential equations in time and an algebraic equation at each spatial mesh point. The differential equations for $C(j\Delta x, t)$, $T_f(j\Delta x, t)$, and $T_c(j\Delta x, t)$, $j = 1, 2, \dots, J$, are solved numerically by a simple, one-step explicit-integration technique, Euler's method.⁴⁸ With these variables computed for the next time step, the value of neutron flux is obtained by solving the matrix equation for that time step. This process continues until the solution is obtained for the desired time interval. The results presented in this section were obtained for $\Delta x = L/50$, where $L(\text{cm})$ is the height of the reactor, and $\Delta t = 0.01$ sec.

Initial conditions for these problems were obtained by using the quasi-linearization procedure to determine the steady-state conditions. However, due to the difference in numerical techniques between the quasi-linearization program and the above finite-difference method, it was necessary to make a slight change in the steady-state conditions. The reactor power level was increased by 2.8% from the initial design conditions given in Ch. III to maintain the criticality conditions. Again, a value of $\mu = 10^{-4}$ was used for the convergence criterion, and the gradient of the system variables was obtained by the finite-difference technique using $\delta a = 10^{-8}$. For the one-dimensional search, the Gauss-Newton technique was used with Search A, while Search B was used for the other techniques.

The first example consisted of selecting a perturbation with $a_1 = a_2 = 1.0$ and $\Sigma'(x) = 1.0 \times 10^{-6}$ for reactor core and blanket regions. This cross-section perturbation resulted in a change of neutron-flux level at the centerline with approximately a 19-sec period. Neutron-flux

measurements are made at 0.2-sec intervals for 1 sec at three spatial points in the core region. With initial estimates of 0.5 and 0.4 for a_1 and a_2 , respectively, the resulting identification is shown in Table XVI.

TABLE XVI. Identification of Parameters for Nonlinear Nuclear Reactor Model

Method	GN	CG	CGM	VM	VMM
a_1	1.0002	1.0001	1.0001	1.0092	1.0001
a_2	0.99989	0.99995	0.99995	0.98804	0.99995
$Q(10^{10})$	0.7832	0.7939	0.7939	408.6	0.7939
Number of Iterations	4	5	5	15 ^a	8
Number of PDE Solutions	15	43	43	121	65

^aNonconvergent after 15 iterations

These solutions again show the efficiency and accuracy of the Gauss-Newton technique in comparison with the conjugate-gradient and variable-metric techniques. Further analysis with various initial estimates yielded similar results, with the solution obtained in four or five iterations by the Gauss-Newton method when the initial estimates were in error by several hundred percent.

The next set of transients to be analyzed were based upon region-dependent reactivity insertions. This type of transient can be interpreted as simulating the control-rod withdrawal from a reactor core if the regions are sufficiently divided. Although only three regions are considered in this analysis, the extension to more regions is trivial. Neutron-flux measurements were obtained for each blanket region in addition to the core measurements, to provide a total twenty-five flux values for a 1-sec interval. Parameters a_1 and a_2 were selected as 1.0, and the value of $\Sigma'(x)$ was selected as 1.0×10^{-6} for positive transients and -1.0×10^{-6} for negative ones. With initial estimates of 3.0 and 1.5 for a_1 and a_2 , respectively, convergent solutions were obtained in four iterations in each case, with fifteen equation solutions when the Gauss-Newton technique was employed. Results are given in Table XVII.

The accuracy and efficiency of the analysis of the transient conditions for the reactor model show that the gradient techniques provide a possible method for performing control-rod calibration and reactivity measurements in a reactor system.

TABLE XVII. Parameter Identification for Spatially Dependent Reactor Transients

Case	1	2	3	4	5
Transient	Positive	Positive	Negative	Negative	Negative
Regions	Core	Core Blanket	Core	Core Blanket	Blanket Core Blanket
a_1	0.99971	0.9997	1.0	1.0004	1.0
a_2	1.0004	1.0	0.99985	0.99912	0.99989
$Q(10^9)$	0.1209	0.1270	0.0716	1.635	0.1373

E. Discussion of Results

The quasi-Newton gradient techniques developed in Ch. IV have been applied to the parameter-identification problem in distributive-parameter models of physical processes that are encountered in the analysis of nuclear reactor systems. Specifically, the Gauss-Newton, conjugate-gradient, and variable-metric techniques were shown to be effective methods for identifying parameters in heat transfer, fluid flow, and nuclear reactor core models.

Results were obtained for up to three unknown parameters in a single parabolic equation which illustrate heat-transfer and fluid-flow processes. Parameters containing heat-transfer coefficients were identified for a set of coupled hyperbolic equations which modeled the transient response of a countercurrent heat exchanger when a step change in temperature was made for one of the fluids. The final example presented was a space- and time-dependent model of an LMFBR which was analyzed to determine the magnitude of step and ramp changes in cross-section values. With the exception of the identification of a single unknown parameter, the Gauss-Newton technique was the most efficient and accurate of the gradient techniques.

The difference in the efficiencies of the gradient techniques are due to the computational requirements of determining the search directions for each technique. At each iteration, all techniques require an evaluation of the criterion function and its derivatives with respect to M unknown parameters. In addition, at each iteration the Gauss-Newton technique requires the solution of a matrix equation to obtain the search directions. For the conjugate-gradient and variable-metric techniques, a one-dimensional search, which on the average required four additional evaluations of the criterion function, is needed at each iteration to determine the search directions. In a distributive-parameter system, each evaluation of the criterion function requires the solution of the system partial differential equations. Since computational time for solving the matrix equation is negligible when compared with the time required for solution of the partial differential equation, the Gauss-Newton method is more efficient for the distributive-parameter system. An opposite result is obtained if the

criterion function is an algebraic equation with dependent variables that are explicitly given. Then computational time is negligible for determining the criterion-function values when compared with the solution of the matrix equations, and thus the conjugate-gradient and variable-metric techniques are more efficient for algebraic-function optimization.

Another asset of the Gauss-Newton technique for distributive-parameter systems occurs when constraints are placed upon the parameter values. For the conjugate-gradient and variable-metric techniques, these parameter constraints may cause erroneous search directions when the constraints prevent the successive search directions from being conjugate, that is, satisfying Eq. 76. Therefore, it is necessary to perform the additional tests given in Sect. IV.F to prevent these erroneous search directions. But the Gauss-Newton requires less stringent conditions to determine the search directions, and parameter constraints can easily be incorporated into this technique.

Although this analysis was limited to identifying a small number of unknown parameters, the results are easily extended to a larger number of unknowns. It is expected that the Gauss-Newton technique would still be the superior method, since the computational time for matrix inversion would still be negligible when compared with the solution of partial differential equations, even if the number of unknowns were to a higher number, such as, twenty. The choice of one independent spatial variable was made to reduce the computational effort, but the gradient techniques are independent of the number of spatial dimensions and, thus, the techniques can be extended to more complicated models.

In summary, the quasi-Newton gradient techniques have been shown to be effective methods for parameter identification of distributive-parameter models of nuclear reactor systems. In particular, the Gauss-Newton technique was shown to be the most efficient and reliable method of obtaining parameter values. Computational time for the examples presented in the chapter required less than 1 min on the IBM 360 computer to obtain the parameter values when the Gauss-Newton technique was used.

VI. CONCLUSIONS AND RECOMMENDATIONS

Application of several methods of parameter identification has been accomplished for lumped- and distributive-parameter systems that are associated with nuclear reactor systems. Specifically, algorithms have been developed for adjusting parameter values from an initial estimate to a set that minimizes a criterion function using simulated system measurements. Results of the analysis show that for both types of systems the unknown parameters can be identified accurately and efficiently.

For the nonlinear, spatially dependent, lumped-parameter model of a nuclear reactor system, the quasi-linearization technique accurately identified the unknown temperature-feedback coefficients. Excellent results were obtained when initial estimates of the unknown parameters were in error by several orders of magnitude; the convergence to the solution was very efficient. In the distributive-parameter models of the nuclear reactor and other heat-transfer and fluid-flow systems, three quasi-Newton gradient techniques were used to identify the unknown parameters. From the results presented for the representative distributive-parameter problems, the Gauss-Newton technique was shown to be the most efficient and accurate gradient technique when compared with the conjugate-gradient and variable-metric techniques.

Computational times for the quasi-linearization technique were about 10 sec for the nuclear reactor model studied. Accurate results were obtained for all the distributive-parameter models in less than 1 min using the Gauss-Newton techniques. For the other two gradient techniques, solutions were obtained in 3 min or less for the majority of the examples.

Results of this analysis in parameter-identification techniques demonstrated their direct application to other problems encountered in the analysis of nuclear reactor systems. Parameter-identification techniques can be used in the planning of experimental tests of nuclear components. They are utilized in the determination of the location and amount of instrumentation to obtain the desired results from the experiment. Also, these techniques can be employed in the analysis of the experimental data to provide better mathematical models of the physical processes. Due to the numerical efficiencies of these techniques they can be incorporated in the on-line analysis of operating nuclear reactor systems to provide parameter values that affect the control and safety of the plant. Examples of this analysis for nuclear plants would be the determination of control-rod worths and the effects of fuel burnup on the reactivity present in the reactor core.

These are several questions that are unanswered in the application of these parameter-identification techniques. Will the convergence of these techniques be altered when there is a large number of unknown parameters or significant errors in the measurements? If the proposed model does not fit the data well, which techniques are the most efficient and accurate? Is there a method of selecting the weighting function in the criterion function that will improve the accuracy of the results? Also, it may be possible to alter the gradient techniques directly to account for inequality constraints instead of specifying a range of values for the one-dimensional search. Finally, a combination of two or more gradient techniques may yield a superior algorithm for parameter identification.

APPENDIX A. Development of Feedback and Thermal-hydraulic Model*

In nuclear power reactors, large quantities of heat energy are released through the fission process in the reactor core. This heat energy is removed by a coolant flowing through the core and is subsequently converted into electrical energy. The process of transferring the heat from the fuel to the coolant can be treated independently by considering the fission process as an internal heat source, and then developing equations that describe the heat transfer and hydrodynamics of the fuel and the coolant. However, these processes are not independent, since the neutronic characteristics of the reactor are functions of the fuel and coolant temperatures due to density changes, Doppler effect, etc. Thus, to develop effectively a nuclear reactor model, the mechanisms of heat transfer and fluid flow must be adequately described.

In order to remove efficiently the heat generated by fission, the reactor fuel is contained in many small pins or in thin plates separated by a flowing coolant. To describe this heterogeneity completely would be impractical due to the large number of fuel elements. Therefore, the concept of the unit cell is introduced, by which the reactor is considered to be composed of identical cells, each consisting of a fuel pin (or plate) and a surrounding equivalent coolant channel. This analysis will be based on a core composed of cylindrical fuel pins, as shown in Fig. A.1. This

Fig. A.1.
Top View of Unit-cell
Configuration.

top view of the reactor shows the fuel and clad as the shaded area; the coolant is the clear area. The equivalent unit cell is shown by the superimposed circle. Figure A.2 shows a longitudinal view of the unit cell.

For this unit cell, temperature distributions in the fuel and coolant can be calculated from basic heat-transfer relations and by considering the fission process as an internal heat source. From these calculated temperature distributions, spatially averaged values in the r -direction are obtained and used to represent the fuel and coolant temperatures at the point where the unit cell is located. The following basic assumptions are used in this analysis:

*The model formulation closely follows that of Ref. 51.

Fig. A.2.
Longitudinal View of Unit-cell
Configuration.

- Properties of the fuel, clad, and coolant are constant in the r -direction.
- The heat source (flux) in the fuel pin of a unit cell is uniformly distributed in the r -direction. The neutron flux is considered flat since the self-shielding effect is minimal in a fast reactor due to small values for the fission cross section.
- There is no heat conduction in the axial (x) direction since most of the heat is transferred horizontally to the coolant.
- The temperature profile is uniform in the coolant in the direction perpendicular to the coolant flow. Since the flow is turbulent in the normal condition, this is also justified.

With these assumptions the temperature distributions are obtained by making an energy balance in each region of the unit cell.

For the fuel region,

$$\rho_f C_{pf} \frac{\partial T_f(r, x, t)}{\partial t} = k_f \nabla_r^2 T_f(r, x, t) + Q_f(r, x, t) . \quad (A.1)$$

In the clad region,

$$\rho_e C_{pe} \frac{\partial T_e(r, x, t)}{\partial t} = k_e \nabla_r^2 T_e(r, x, t) . \quad (A.2)$$

In the coolant region,

$$\begin{aligned} \rho_c C_{pc} \frac{\partial T_c(x,t)}{\partial t} &= -v_c \rho_c C_{pc} \frac{\partial T_c(x,t)}{\partial x} \\ &+ \frac{2h_c r_2}{(r_3^2 - r_2^2)} [T_e(r_2, x, t) - T_c(x, t)] . \end{aligned} \quad (A.3)$$

where

- f, e, c - subscripts referring to fuel, clad, and coolant, respectively,
- r - radial space variable with respect to the unit cell,
- r_1, r_2, r_3 - values of r at the fuel-clad interface, clad-coolant interface, and unit-cell boundary, respectively,
- T_i - temperature of material i,
- ρ_i - density of material i,
- C_{pi} - heat capacity of material i,
- v_c - coolant velocity,
- h_c - heat-transfer coefficient between the clad and coolant,
- k_i - thermal conductivity in material i,
- $Q_f(r, x, t)$ - volumetric heat source in the fuel,
- x - axial reactor coordinate and direction of coolant flow.

The boundary conditions for these equations are

$$\left. \frac{\partial T_f(r, x, t)}{\partial r} \right|_{r=0} = 0 ; \quad (A.4)$$

$$T_c(x, t) \Big|_{x=0} = T_f(r, x, t) \Big|_{x=0} = T_a ; \quad (A.5)$$

$$\begin{aligned} -k_f \left. \frac{\partial T_f(r, x, t)}{\partial r} \right|_{r=r_1} &= h_e [T_f(r_1, x, t) - T_e(r_1, x, t)] \\ &= -k_e \left. \frac{\partial T_e(r, x, t)}{\partial r} \right|_{r=r_1} ; \end{aligned} \quad (A.6)$$

$$-k_e \frac{\partial T_e(r, x, t)}{\partial r} \bigg|_{r=r_2} = h_c [T_e(r_2, x, t) - T_c(x, t)] , \quad (\text{A.7})$$

where T_c is the ambient temperature and h_c is the heat-transfer coefficient between the fuel and clad.

Equations for the average temperature for each material in the unit cell are obtained by multiplying Eqs. A.1 and A.2 by $2\pi r dr$ and integrating over the region with material i (region R_i). The average temperature in region R_i is defined as

$$\bar{T}_i(x, t) = \frac{1}{A_i} \int_{R_i} 2\pi r T_i(r, x, t) dr , \quad (\text{A.8})$$

and the average volumetric heat source is defined as

$$\bar{Q}_f(x, t) = \frac{1}{A_f} \int_{R_f} 2\pi r Q_f(r, x, t) dr , \quad (\text{A.9})$$

where A_i is the cross-sectional area of region R_i . The resulting equations for the average fuel and clad temperatures are

$$\rho_f C_{pf} \frac{\partial \bar{T}_f(x, t)}{\partial t} = \frac{2h_e}{r_1} [T_e(r_1, x, t) - T_f(r_1, x, t)] + \bar{Q}_f(x, t) \quad (\text{A.10})$$

and

$$\begin{aligned} \rho_e C_{pe} \frac{\partial \bar{T}_e(x, t)}{\partial t} &= \frac{2r_2 h_c}{(r_2^2 - r_1^2)} [T_c(x, t) - T_e(r_1, x, t)] \\ &+ \frac{2k_e r_1 h_e}{k_f (r_2^2 - r_1^2)} [T_f(r_1, x, t) - T_e(r_1, x, t)] . \end{aligned} \quad (\text{A.11})$$

Equations A.3, A.10, and A.11 can be simplified by assuming negligible heat storage in the clad. Thus, Eq. A.2 becomes

$$k_e \nabla_r^2 T_e(r, x, t) = 0 , \quad (\text{A.12})$$

which has a solution of the form

$$T_e(r, x, t) = C_1 \ln r + C_2, \quad (\text{A.13})$$

where C_1 and C_2 are constants to be evaluated at the boundary points of the clad. By use of the results of Eq. A.13, the boundary conditions given by Eqs. A.6 and A.7 become

$$-k_f \left. \frac{\partial T_f(r, x, t)}{\partial r} \right|_{r=r_1} = h[T_f(r_1, x, t) - T_c(x, t)] \quad (\text{A.14})$$

and

$$[T_e(r_2, x, t) - T_c(x, t)]h_c = \frac{r_1}{r_2} h[T_f(r_1, x, t) - T_c(x, t)], \quad (\text{A.15})$$

where h is an equivalent heat-transfer coefficient:

$$h = \frac{1}{r_1} \left[\frac{1}{r_1 h_e} + \frac{1}{r_2 h_c} + \frac{1}{k_e} \ln \frac{r_2}{r_1} \right]^{-1}. \quad (\text{A.16})$$

With these results the heat-transfer model can now be written in terms of $\bar{T}_f(x, t)$ and $T_c(x, t)$:

$$\rho_f C_{pf} \frac{\partial \bar{T}_f(x, t)}{\partial t} = \frac{2h}{r_1} [T_c(x, t) - T_f(r_1, x, t)] + \bar{Q}_f(x, t); \quad (\text{A.17})$$

$$\begin{aligned} \rho_c C_{pc} \frac{\partial T_c(x, t)}{\partial t} &= -v_c \rho_c C_{pc} \frac{\partial T_c(x, t)}{\partial x} \\ &+ \frac{2r_1 h}{(r_3^2 - r_2^2)} [T_f(r_1, x, t) - T_c(x, t)]. \end{aligned} \quad (\text{A.18})$$

The volumetric heat source for the unit cell, $Q(x, t)$ is given by the expression

$$Q(x, t) = \epsilon' \Sigma_f(x) \phi(x, t), \quad (\text{A.19})$$

where ϵ' is the energy released per fission, $\Sigma_f(x)$ is the time-independent homogenized fission cross section, and $\phi(x,t)$ is the neutron flux in the unit cell. A relationship between $Q(x,t)$ and the volumetric heat source in the fuel, $\bar{Q}_f(x,t)$, is given by

$$\bar{Q}_f(x,t) = Q(x,t)r_3^2/r_1^2. \quad (A.20)$$

At steady state the time-independent value of the fuel temperature, $T_f(r_1,x)$, can be written in terms of the average values of $T_f(x)$ and $\bar{Q}_f(x)$:

$$T_f(r_1,x) = \bar{T}_f(x) - \bar{Q}_f(x) \frac{r_1^2}{8k_f}. \quad (A.21)$$

With the assumption that Eq. A.21 is also valid for the time-dependent case and through use of Eqs. A.19 and A.20, the heat-transfer model given by Eqs. A.17 and A.18 becomes

$$\frac{\partial \bar{T}_f(x,t)}{\partial t} = \frac{2h}{r_1 \rho_f C_{pf}} [T_c(x,t) - \bar{T}_f(x,t)] - \frac{\epsilon''}{\rho_f C_{pf}} \Sigma_f(x) \phi(x,t); \quad (A.22)$$

$$\begin{aligned} \frac{1}{v_c} \frac{\partial T_c(x,t)}{\partial t} &= - \frac{\partial T_c(x,t)}{\partial x} + \frac{h'}{r_1 v_c \rho_c C_{pc}} [\bar{T}_f(x,t) - T_c(x,t)] \\ &\quad - \frac{\eta h'}{r_1 v_c \rho_c C_{pc}} \Sigma_f(x) \phi(x,t), \end{aligned} \quad (A.23)$$

where

$$\epsilon'' = \epsilon' \frac{r_3^2}{r_1^2} \left[1 + \frac{r_1 h}{4k_f} \right];$$

$$h' = 2r_1^2 h / (r_3^2 - r_2^2);$$

$$\eta = \epsilon' r_3^2 / 8k_f.$$

The initial conditions for Eqs. A.22 and A.23 are

$$T_c(x,t) \Big|_{t=0} = T_{c0}(x) \quad (A.24)$$

and

$$\bar{T}_f(x,t) \Big|_{t=0} = \bar{T}_{f0}(x) , \quad (A.25)$$

and the boundary conditions are

$$T_c(x,t) \Big|_{x=0} = \bar{T}_f(x,t) \Big|_{x=0} = T_a . \quad (A.26)$$

The steady-state or time-independent equations for the model given by Eqs. A.22 and A.23 are obtained by setting $\partial T_c(x,t)/\partial t$ and $\partial \bar{T}_f(x,t)/\partial t$ equal to zero. The resulting equations are

$$\bar{T}_f(x) = T_c(x) + \xi \Sigma_f(x) \phi(x) \quad (A.27)$$

and

$$\frac{dT_c(x)}{dx} = \epsilon \Sigma_f(x) \phi(x) , \quad (A.28)$$

where

$$\xi = \epsilon'' r_1 / 2h \quad (A.29)$$

and

$$\epsilon = \frac{h' \left(\epsilon'' \frac{r_1}{2h} - \eta \right)}{r_1 v_c \rho_c C_{pc}} \quad (A.30)$$

The thermohydraulic parameters for the LMFBR were obtained from a fast reactor parameter study⁵¹ and are given in Table A.1.

To incorporate the effects of temperature changes into the neutronics of the nuclear reactor, variations in neutronic cross sections will be employed. The following equation shows the linear dependence based on a two-term Taylor series expansion for a system macroscopic cross section, $\Sigma(T_f, T_c)$:

TABLE A.I. Thermohydraulic Parameters

Parameter	Value
r_1	0.2851 cm
r_2	0.3573 cm
r_3	0.5235 cm
ρ_f	8.39 g/cm ³
ρ_c	0.8195 g/cm ³
C_{pf}	0.355 W-sec/g-°C
C_{pc}	1.256 W-sec/g-°C
ϵ'	3.2×10^{-11} W-sec/fission
k_f	0.0234 W/cm-°C
k_e	0.2250 W/cm-°C
h_e	0.852 W/cm ² -°C
h_c	11.36 W/cm ² -°C
v_c	492.6 cm/sec

$$\underline{\Sigma}(\bar{T}_f, T_c) = \underline{\Sigma}(\bar{T}_{f0}, T_{c0}) + \frac{\partial \underline{\Sigma}}{\partial \bar{T}_f} [\bar{T}_f - \bar{T}_{f0}] + \frac{\partial \underline{\Sigma}}{\partial T_c} [T_c - T_{c0}] , \quad (A.31)$$

where

- $\bar{T}_f, T_c$ - fuel and coolant temperatures,
- $\bar{T}_{f0}, T_{c0}$ - reference fuel and coolant temperatures,
- $\frac{\partial \underline{\Sigma}}{\partial \bar{T}_f}, \frac{\partial \underline{\Sigma}}{\partial T_c}$ - first-order fuel and coolant temperature effect on a system macroscopic cross section.

The dependence of Σ , $\bar{T}_f$, and T_c on time and space are not shown. The system macroscopic cross section is a vector quantity which includes absorption, fission, and scattering cross sections. In general, temperature coefficients are space- and time-dependent, but in this analysis they will be treated as constants. The following equations define the fuel and coolant temperature coefficients for the fission and absorption cross sections:

$$a_f = \frac{1}{\Sigma_f(\bar{T}_{f0}, T_{c0})} \frac{\partial \Sigma_f}{\partial \bar{T}_f} ; \quad (A.32)$$

$$a_c = \frac{1}{\Sigma_f(\bar{T}_{f0}, T_{c0})} \frac{\partial \Sigma_f}{\partial T_c} ; \quad (A.33)$$

$$a'_f = \frac{1}{\Sigma_a(\bar{T}_{f0}, T_{c0})} \frac{\partial \Sigma_a}{\partial \bar{T}_f} ; \quad (A.34)$$

$$a'_c = \frac{1}{\Sigma_a(\bar{T}_{f0}, T_{c0})} \frac{\partial \Sigma_a}{\partial T_c} . \quad (A.35)$$

The temperature-dependent fission and absorption cross sections can now be written as

$$\Sigma_f(\bar{T}_f, T_c) = \Sigma_f(\bar{T}_{f0}, T_{c0}) [1.0 + a_f(\bar{T}_f - \bar{T}_{f0}) + a_c(T_c - T_{c0})] \quad (A.36)$$

and

$$\Sigma_a(\bar{T}_f, T_c) = \Sigma_a(\bar{T}_{f0}, T_{c0}) [1.0 + a'_f(\bar{T}_f - \bar{T}_{f0}) + a'_c(T_c - T_{c0})] . \quad (A.37)$$

APPENDIX B. Development of Newton and Gauss-Newton Gradient Techniques

Newton's method is developed by using a second-order Taylor series expansion of the criterion function about its minimum value, $\underline{a}^*$. The M-dimensional vector $\underline{a}^*$ is the solution of the identification problem. The value of the criterion function at any point $\underline{a}$ is approximated by

$$Q(\underline{a}) = Q(\underline{a}^*) + \frac{\partial Q(\underline{a}^*)^T}{\partial \underline{a}} [\underline{a} - \underline{a}^*] + \frac{1}{2} \left[\underline{a} - \underline{a}^* \right]^T \frac{\partial^2 Q(\underline{a}^*)}{\partial \underline{a} \partial \underline{a}^T} [\underline{a} - \underline{a}^*] . \quad (\text{B.1})$$

The values for the gradient vector and the second-derivative matrix of the criterion function are evaluated at $\underline{a}^*$. If Eq. B.1 is differentiated with respect to $\underline{a}$, the following expression is obtained,

$$\frac{\partial Q(\underline{a})}{\partial \underline{a}} = \frac{\partial Q(\underline{a}^*)}{\partial \underline{a}} + \frac{\partial^2 Q(\underline{a}^*)}{\partial \underline{a} \partial \underline{a}^T} [\underline{a} - \underline{a}^*] . \quad (\text{B.2})$$

Since the gradient of the criterion function is zero at its minimum, the solution for the values of $\underline{a}^*$ is given by

$$\underline{a}^* = \underline{a} - \left[\frac{\partial^2 Q(\underline{a}^*)}{\partial \underline{a} \partial \underline{a}^T} \right]^{-1} \frac{\partial Q(\underline{a})}{\partial \underline{a}} . \quad (\text{B.3})$$

Thus, the solution of the identification problem can be obtained from any value of $\underline{a}$ provided that the Taylor series expansion given by Eq. B.1 is a valid representation of the criterion function at $\underline{a}$. When the criterion function is explicitly quadratic in $\underline{a}$, the second-derivative matrix is constant for all $\underline{a}$, and one-step convergence occurs. The criterion function of the distributive-parameter identification problem is implicit in $\underline{a}$, and in general the second derivative of the criterion function will not be constant.

When the criterion function is not explicitly quadratic in $\underline{a}$, Eq. B.3 can be used as a basis for an iterative relation to obtain the solution of the identification problem. The iterative relation is given by

$$\underline{a}_{i+1} = \underline{a}_i - \left[\frac{\partial^2 Q(\underline{a}_i)}{\partial \underline{a} \partial \underline{a}^T} \right]^{-1} \frac{\partial Q(\underline{a}_i)}{\partial \underline{a}} . \quad (\text{B.4})$$

To simplify the notation the following terms are defined:

$$\underline{g}_i = \frac{\partial Q(\underline{a}_i)}{\partial \underline{a}} \quad (\text{B.5})$$

and

$$\underline{G}_i = \frac{\partial^2 Q(\underline{a}_i)}{\partial \underline{a} \partial \underline{a}^T} \quad (\text{B.6})$$

Equation B.4 now can be written as

$$\underline{a}_{i+1} = \underline{a}_i - \underline{G}_i^{-1} \underline{g}_i \quad (\text{B.7})$$

In the vicinity of the minimum, Eq. B.7 will yield a value of $\underline{a}_{i+1}$ which satisfies the descent property

$$Q(\underline{a}_{i+1}) < Q(\underline{a}_i) \quad (\text{B.8})$$

If the initial estimate of the unknown parameters is not within the neighborhood of the solution, a one-dimensional search for ρ_i is performed in order to satisfy Eq. B.8. The iterative relationship for Newton's method is then given by

$$\underline{a}_{i+1} = \underline{a}_i - \rho_i \underline{G}_i^{-1} \underline{g}_i \quad (\text{B.9})$$

The Gauss-Newton technique is an attempt to obtain convergence characteristics that are similar to Newton's method without calculating the second derivative of the criterion function with respect to $\underline{a}$. A first-order Taylor series expansion of the system variables is made about an initial value $\underline{a}_0$ to yield a set of equations:

$$\underline{u}(\underline{x}, t, \underline{a}) = \underline{u}(\underline{x}, t, \underline{a}_0) + \frac{\partial \underline{u}(\underline{x}, t, \underline{a}_0)}{\partial \underline{a}}^T [\underline{a} - \underline{a}_0] \quad (\text{B.10})$$

where $\underline{u}(\underline{x}, t, \underline{a}_0)$ denotes the value of the system variables obtained by using the value of $\underline{a}_0$ for the unknown parameters. This result is substituted into the criterion function:

$$Q = \sum_{r=1}^R \sum_{s=1}^S \left\{ y(\underline{x}_r, t_s) - \underline{u}(\underline{x}_r, t_s, \underline{a}) \right\}^2 \quad (\text{B.11})$$

to obtain a first-order approximation for the criterion function:

$$Q = \sum_{r=1}^R \sum_{s=1}^S \left\{ y(x_r, t_s) - u(x_r, t_s, \underline{a}) - \frac{\partial u(x_r, t_s, \underline{a}_0)^T}{\partial \underline{a}} [\underline{a} - \underline{a}_0] \right\}^2. \quad (\text{B.12})$$

Taking the partial of Q with respect to $\underline{a}$ forms a set of M equations when $\partial Q / \partial \underline{a}$ is set equal to zero:

$$\sum_{r=1}^R \sum_{s=1}^S \left\{ \frac{\partial u(x_r, t_s, \underline{a}_0)^T}{\partial \underline{a}} [y(x_r, t_s) - u(x_r, t_s, \underline{a}_0)] \right\} = \sum_{r=1}^R \sum_{s=1}^S \left\{ \frac{\partial u(x_r, t_s, \underline{a}_0)^T}{\partial \underline{a}} \frac{\partial u(x_r, t_s, \underline{a}_0)}{\partial \underline{a}} [\underline{a} - \underline{a}_0] \right\}. \quad (\text{B.13})$$

This equation can be formulated as a matrix equation of the form

$$\frac{\partial u(\underline{a}_0)^T}{\partial \underline{a}} \frac{\partial u(\underline{a}_0)}{\partial \underline{a}} [\underline{a} - \underline{a}_0] = \frac{\partial u(\underline{a}_0)^T}{\partial \underline{a}} [y - u(\underline{a}_0)], \quad (\text{B.14})$$

where $\partial u(\underline{a}_0) / \partial \underline{a}$ is an $N'RS$ by M matrix and $[y - u(\underline{a}_0)]$ is an $N'RS$ column vector, with N' being the number of variables that are measured and used in the criterion function. The resulting solution for $(\underline{a} - \underline{a}_0)$ is given by

$$\underline{a} - \underline{a}_0 = \left[\frac{\partial u(\underline{a}_0)^T}{\partial \underline{a}} \frac{\partial u(\underline{a}_0)}{\partial \underline{a}} \right]^{-1} \frac{\partial u(\underline{a}_0)^T}{\partial \underline{a}} [y - u(\underline{a}_0)]. \quad (\text{B.15})$$

If Eq. B.11 is differentiated with respect to $\underline{a}$ to form the gradient of the criterion function, Eq. B.15 can be written as

$$\underline{a} - \underline{a}_0 = -\frac{1}{2} \left[\frac{\partial u(\underline{a}_0)^T}{\partial \underline{a}} \frac{\partial u(\underline{a}_0)}{\partial \underline{a}} \right]^{-1} \underline{g}_0. \quad (\text{B.16})$$

Upon comparison of Eqs. B.4 and B.16, the second derivative matrix in Newton's method is found to be approximated by

$$G \approx 2 \left[\frac{\partial u(\underline{a}_0)^T}{\partial \underline{a}} \frac{\partial u(\underline{a}_0)}{\partial \underline{a}} \right] \quad (\text{B.17})$$

in the Gauss-Newton method.

Equation B.16 can be used to form a basis for an iterative relationship to determine the unknown parameters by

$$\underline{a}_{i+1} = \underline{a}_i - \left[\frac{\partial u(\underline{a}_i)^T}{\partial \underline{a}} \frac{\partial u(\underline{a}_i)}{\partial \underline{a}} \right]^{-1} \underline{g}_i . \quad (\text{B.18})$$

Similar to Newton's method, Eq. B.18 will satisfy the descent property, Eq. B.8, in the vicinity of the solution. But if the initial estimates of the unknown parameters are not in the neighborhood of the solution, a one-dimensional search for ρ_i is required to satisfy Eq. B.8. The Gauss-Newton iterative relationship is then given by

$$\underline{a}_{i+1} = \underline{a}_i - \rho_i \left[\frac{\partial u(\underline{a}_i)^T}{\partial \underline{a}} \frac{\partial u(\underline{a}_i)}{\partial \underline{a}} \right]^{-1} \underline{g}_i . \quad (\text{B.19})$$

APPENDIX C. Method of Conjugate Directions

Both the conjugate-gradient and variable-metric techniques are based on the fact that the criterion function can be adequately approximated by a quadratic function. Consider the following quadratic function about the minimum value of $\underline{a}^*$:

$$Q(\underline{a}) = Q(\underline{a}^*) + \underline{\ell}^T [\underline{a} - \underline{a}^*] + \frac{1}{2} [\underline{a} - \underline{a}^*] \underline{S} [\underline{a} - \underline{a}^*] , \quad (C.1)$$

where $\underline{a}$ is an M-dimensional variable, $\underline{\ell}$ is a Mth-order column vector of constant coefficients, and $\underline{S}$ is a M by M positive-definite matrix of constant coefficients. Restricting the $\underline{S}$ matrix to be positive-definite insures that a relative minimum exists for $Q(\underline{a})$. The gradient of the quadratic function with respect to $\underline{a}$ is given by the Mth-order vector

$$\underline{g} = \frac{\partial Q(\underline{a})}{\partial \underline{a}} = \underline{\ell} + \underline{S} [\underline{a} - \underline{a}^*] . \quad (C.2)$$

The upgrading of the $\underline{a}$ values from the present iteration to the next iteration is based on the following relation:

$$\underline{a}_{i+1} = \underline{a}_i + \rho_i \underline{d}_i , \quad (C.3)$$

where $\underline{d}_i$ is the M-dimensional direction vector and ρ_i is the distance moved along $\underline{d}_i$. Through use of Eq. C.3 the value of the criterion function at $\underline{a}_{i+1}$ is found to have the form

$$Q(\underline{a}_{i+1}) = Q(\underline{a}_i + \rho_i \underline{d}_i) . \quad (C.4)$$

The minimum of $Q(\underline{a}_{i+1})$ along the search direction $\underline{d}_i$ occurs when

$$\frac{dQ(\underline{a}_i + \rho_i \underline{d}_i)}{d\rho_i} = 0 , \quad (C.5)$$

which implies that

$$\underline{g}_{i+1}^T \underline{d}_i = 0 . \quad (C.6)$$

Thus, the gradient at $\underline{a}_{i+1}$ is orthogonal to the previous search direction when Eq. C.5 is satisfied.

Successive values of the gradient can be obtained from Eq. C.5:

$$\underline{g}_{i+1} = \underline{g}_i + \underline{S}[\underline{a}_{i+1} - \underline{a}_i] . \quad (C.7)$$

Substituting Eq. C.3 into Eq. C.7 relates the successive iterative values of the gradient to the search direction:

$$\underline{g}_{i+1} = \underline{g}_i + \underline{S}\rho_i \underline{d}_i . \quad (C.8)$$

By using Eqs. C.6 and C.8 an explicit value for ρ_i can be obtained:

$$\rho_i = - \frac{\underline{g}_i^T \underline{d}_i}{\underline{d}_i^T \underline{S} \underline{d}_i} . \quad (C.9)$$

Since $\underline{S}$ is positive-definite, a value for ρ_i can be obtained provided that

$$\underline{g}_i^T \underline{d}_i \neq 0 . \quad (C.10)$$

When Eq. C.8 is used repeatedly, the k^{th} value of the gradient can be related to any previous j^{th} value by

$$\underline{g}_k = \underline{g}_j + \sum_{i=j}^{k-1} \underline{S}\rho_i \underline{d}_i \quad \text{for } 0 \leq j \leq k-1. \quad (C.11)$$

If the transpose of Eq. C.11 is postmultiplied by $\underline{d}_j$ and the value for ρ_j determined by Eq. C.9 is used, then

$$\underline{g}_k^T \underline{d}_j = \sum_{i=j+1}^{k-1} \underline{S}\rho_i \underline{d}_i^T \underline{d}_j \quad \text{for } 0 \leq j \leq k-2. \quad (C.12)$$

If the search directions $\underline{d}_i$ are S-conjugate with respect to the previous search directions $\underline{d}_j$, that is,

$$\underline{d}_i^T \underline{S} \underline{d}_j = 0 \quad \text{for } 0 \leq j < i \leq k-1 , \quad (C.13)$$

then Eq. C.12 becomes

$$\underline{g}_k^T \underline{d}_j = 0 \quad \text{for } 0 \leq j \leq k-2. \quad (C.14)$$

For the $(k - 1)^{\text{th}}$ iteration, Eq. C.6 requires that

$$\underline{g}_k^T \underline{d}_{k-1} = 0. \quad (\text{C.15})$$

Combining Eqs. C.14 and C.15 yields

$$\underline{g}_k^T \underline{d}_j = 0 \quad \text{for } 0 \leq j \leq k - 1. \quad (\text{C.16})$$

When $k = M$, Eq. C.16 becomes

$$\underline{g}_M^T \underline{d}_j = 0 \quad \text{for } 0 \leq j \leq M - 1. \quad (\text{C.17})$$

Since the sequence of $\underline{d}_i$, $i = 0, 1, 2, \dots, M - 1$, is a set of nonzero, linearly independent directions, they form a complete basis in M -dimensional $\underline{a}$ space. Thus, the solution for the minimum of the quadratic function can be written as a linear combination of these search directions. Since the directions of $\underline{d}_i$ form a complete basis, the minimum of the criterion function is obtained in M iterations provided that the criterion function is explicitly quadratic in $\underline{a}$. Convergence for the criterion function given by Eq. 4.6 cannot be guaranteed in M iterations due to its implicit dependence on the unknown parameters.

The conjugate-gradient method is one of the simplest ways of obtaining a set of search directions that are conjugate with respect to the second derivative of the criterion function. For the conjugate-gradient method the search sequence is given by

$$\underline{d}_0 = -\underline{g}_0 \quad (\text{C.18})$$

and

$$\underline{d}_i = -\underline{g}_i + \frac{\underline{g}_i^T \underline{g}_i}{\underline{g}_{i-1}^T \underline{g}_{i-1}} \underline{d}_{i-1} \quad \text{for } i \geq 1. \quad (\text{C.19})$$

Proof of the convergence properties of this search sequence is given by Beckman,⁵⁸ who generated the above set of directions by means of a "Gram-Schmidt" orthogonalization procedure to obtain the set of M linearly independent vectors.

The variable-metric method was first proposed by Davidon⁶⁰ and was reformulated by Fletcher and Powell⁶¹ to insure that the M by M -dimensional $\underline{H}_i$ matrix in the search direction vector,

$$\underline{d}_i = -\underline{H}_i \underline{g}_i, \quad (\text{C.20})$$

remained symmetric and positive-definite. The $\underline{H}_1$ matrix is chosen such that the value of the matrix after M iterations is equal to the inverse of the second-derivative matrix. With the search directions given by Eq. C.20, the $\underline{H}_1$ is chosen to be

$$\underline{H}_0 = \underline{I} ; \quad (C.21)$$

$$\underline{H}_i = \underline{H}_{i-1} + \frac{\Delta \underline{a}_{i-1} \Delta \underline{a}_{i-1}^T}{\Delta \underline{a}_{i-1}^T \Delta \underline{g}_{i-1}} - \frac{\underline{H}_{i-1} \Delta \underline{g}_{i-1} \Delta \underline{g}_{i-1}^T \underline{H}_{i-1}}{\Delta \underline{g}_{i-1}^T \underline{H}_{i-1} \Delta \underline{g}_{i-1}} , \quad (C.22)$$

with

$$\Delta \underline{a}_{i-1} = \underline{a}_i - \underline{a}_{i-1} \quad (C.23)$$

and

$$\Delta \underline{g}_{i-1} = \underline{g}_i - \underline{g}_{i-1} . \quad (C.24)$$

For an explicitly quadratic function the variable-metric method will yield a solution in M iterations with the value of $\underline{H}_1$ after iteration M equal to the inverse of the second derivative of the criterion function with respect to the unknown parameters. Proof of the convergence properties is given by Fletcher and Powell.⁶¹

ACKNOWLEDGMENTS

The author wishes to express his gratitude to his Argonne advisor, Dr. Chun Hsu, for his patience and assistance and to his university advisor, Dr. Dale Metcalf, for his guidance and support throughout the period of this work. The assistance and suggestions of the staff of Argonne National Laboratory, especially Dr. Loren Habegger, were greatly appreciated. Also, the author wishes to acknowledge the Argonne University Association and Argonne National Laboratory for their financial assistance and facilities to perform this research. The financial support offered by the University of Virginia and the United States Atomic Energy Commission in the form of Traineeships during the author's residence at the University is gratefully appreciated.

REFERENCES

1. R. C. K. Lee, *Optimal Estimation, Identification, and Control*, The M.I.T. Press, Cambridge, Mass. (1964).
2. M. Cuenod and A. P. Sage, *Comparisons of Some Methods Used for Process Identification*, *Automatica*, 4(4), 235-268 (1968).
3. J. J. D'Azzo and C. H. Houpis, *Feedback Control System Analysis and Synthesis*, McGraw-Hill Book Co., Inc., New York (1960).
4. M. Cuenod and A. E. Durling, *An Introduction to Impulse Analysis*, Academic Press, New York (1967).
5. V. W. Eveleigh, *Adaptive Control and Optimization Techniques*, McGraw-Hill Book Co., Inc., New York (1967).
6. *Special Issue on Fast Fourier Transform and its Application to Digital Filtering and Spectral Analysis*, IEEE Transactions on Audio and Electro-Acoustics, AV-15 (1967).
7. M. J. Box, D. Davies, and W. H. Swaan, *Nonlinear Optimization Techniques*, I.C.I. Monograph No. 5, Oliver and Boyd, Edinburgh (1969).
8. P. D. Flanagan, P. A. Vitale, and J. Mendelsohn, *A Numerical Investigation of Several One-Dimensional Search Procedures in Nonlinear Regression Problems*, *Technometrics*, 11(2), 265-284 (1969).
9. D. J. Wilde and C. S. Beightler, *Foundations of Optimization*, Prentice-Hall, Englewood Cliffs, New Jersey (1967).
10. C. B. Tompkins, "Methods of Steepest Descent," in *Modern Mathematics for the Engineer*, edited by E. F. Bechenback, McGraw-Hill Book Co., Inc., New York (1956).
11. R. Fletcher, "A Review of Methods for Unconstrained Optimization," in *Optimization*, edited by R. Fletcher, Academic Press, New York (1969).
12. M. J. D. Powell, "Minimization of Function of Several Variables," in *Numerical Analysis: An Introduction*, edited by J. Walsh, Thompson Book Co., Washington, D.C. (1967).
13. Y. Bard, *Comparison of Gradient Methods for the Solution of Nonlinear Parameter Estimation Problems*, *SIAM Journal of Numerical Analysis*, 7(1), 157-186 (1970).
14. W. B. Davenport, Jr. and W. L. Root, *Random Signal and Noise*, McGraw-Hill Book Co., Inc., New York (1958).
15. R. E. Kalman, *A New Approach to Linear Filtering and Prediction Problems*, *Trans. ASME, Journal of Basic Engineering*, 82, 35-45 (1960).

16. A. E. Albert and L. A. Gardner, *Stochastic Approximation and Nonlinear Regression*, The M.I.T. Press, Cambridge, Mass. (1967).
17. R. E. Bellman, *Dynamic Programming*, Princeton University Press, Princeton, New Jersey (1957).
18. R. E. Bellman and R. E. Kalaba, *Quasi-linearization and Nonlinear Boundary-Value Problems*, American Elsevier, New York (1965).
19. E. S. Lee, *Quasi-linearization and Invariant Imbedding*, Academic Press, New York (1968).
20. R. E. Bellman and R. E. Kalaba, "Dynamic Programming, Invariant Imbedding, and Quasi-linearization: Comparisons and Interconnections," in *Computing Methods in Optimization Problems*, edited by A. V. Balakrishnan and L. W. Newstadt, Academic Press, New York (1964).
21. P. Kenneth and R. McGill, "Two Point Boundary-Value-Problem Techniques," in *Advances in Control Systems*, 3, edited by C. T. Leondes, Academic Press, New York (1966).
22. W. C. Lipinski, *Optimal Digital Computer Control of Nuclear Reactors*, ANL-7530 (1969).
23. S. P. Sage and T. W. Ellis, "Sequential Suboptimal Adaptive Control of Nonlinear Systems," *Proc. of National Electronic Conference*, 22, 692-697 (1966).
24. A. P. Sage and G. W. Masters, *Identification and Modeling of States and Parameters of Nuclear Reactor Systems*, IEEE Transactions on Nuclear Science, NS-14, 1, 279-285 (1967).
25. L. J. Habegger, *The Use of the Kalman Filter for the Estimation of Nuclear Reactor Parameters*, Ph.D. Dissertation, Purdue University, 1968.
26. L. J. Habegger, R. E. Bailey, and K. Kadavanich, *The Use of Quasi-linearization for the Identification of Nuclear Reactor Parameters*, Trans. ANS, 10(1), 176-177 (1967).
27. L. J. Habegger and C. Hsu, *The Use of Quasi-linearization for the Solution of Nonlinear Space-Dependent Reactor Equations*, Trans. ANS, 12(2), 830-831 (1969).
28. A. C. Robinson, *A Survey of Optimal Control of Distributed Parameter Systems*, Aerospace Research Laboratories Report, ARL 69-0177 (1969).
29. P. K. C. Wang, *Theory of Stability and Control for Distributed Parameter Systems (a Bibliography)*, International Journal of Control, 7(2), 101-116 (1968).
30. B. F. Jones, Jr., *The Determination of a Coefficient in a Parabolic Differential Equation, Part I. Existence and Uniqueness*, J. Math. and Mech, 11(6), 907-918 (1967).

31. J. Douglas, Jr. and B. F. Jones, Jr., *The Determination of a Coefficient in a Parabolic Differential Equation, Part II. Numerical Approximation*, J. Math. and Mech., 11(6), 919-926 (1962).
32. F. J. Perdreauxville and R. E. Goodson, *Identification of Distributed Systems Described by Partial Differential Equations*, Trans. ASME, J. of Basic Eng., 58(2), 463-468 (1966).
33. G. N. Saridis and P. C. Badavas, "Identification of Distributed Parameter Systems by Stochastic Approximation," *Proc. of IEEE 7th. Symposium on Adaptive Processes*, Paper No. 52 (1968).
34. G. A. Phillipson and S. K. Mitter, "Numerical Solution of a Distributed Identification Problem via a Direct Method," in *Computing Methods in Optimization Problems*, edited by A. V. Balakrishman and L. W. Newstadt, Academic Press, New York (1964).
35. J. F. Croce-Spinelli, "A Method for Identification Problems in Partial Differential Equations," *Information Processing 68*, North Holland Publ., Amsterdam, 159-163 (1969).
36. P. L. Collins and H. C. Khatri, *Identification of Distributed Parameter Systems Using Finite Differences*, Trans. of ASME, J. of Basic Eng., 91(2), 239-245 (1969).
37. J. H. Seinfeld, *Identification of Parameters in Partial Differential Equations*, Chem. Eng. Sci., 24, 65-74 (1969).
38. R. J. Herbold, "The Use of Interactive Techniques for Determining Parameters and Physical Constants in Partial Differential Equations," *Proc. of Summer Computer Simulation Conf.*, 214-224 (1970).
39. L. V. Kantorovitch, Doklady Akad. Nauk. S.S.S.R., 59, 1237-1240 (1948) as reported in *Approximation Methods of Higher Analysis* by L. V. Kantorovitch and V. I. Krylov, Wiley (Interscience) Book Co., New York (1958).
40. M. R. Hestenes, *Numerical Methods of Obtaining Solutions of Fixed End Point Problems in the Calculus of Variations*, RAND Corp. Report, RM-102 (1949).
41. R. Bellman, "Functional Equations in the Theory of Dynamic Programming V. Positivity and Quasi-linearity," *Proc. Natl. Acad. Sci. US*, 41, 743-746 (1955).
42. R. Kalaba, *On Nonlinear Differential Equations, the Maximum Operation and Monotone Convergence*, J. Math. and Mech., 8, 519-574 (1959).
43. R. McGill and P. Kenneth, *A Convergence Theorem on the Iterative Solution of Nonlinear Two-Point Boundary Value Systems*, XIVth. International Astronautical Federation Congress, Paris, France (1963).
44. R. E. Bellman, *Successive Approximation and Computer Storage Problems in Ordinary Differential Equations*, Comm. ACM, 4, 222-223 (1961).

45. D. B. Larson, *Identification of Parameters by the Method of Quasi-linearization*, Cornell Aeronautical Laboratory, Report No. CAL-164, 1968.
46. D. Thompson and G. Golden, Private communication, Jan 4, 1967.
47. D. A. Meneley, L. C. Kvitek, and D. M. O'Shea, *MACH-1, A One-dimensional Diffusion Theory Package*, ANL-7223 (1966).
48. S. D. Conte, *Elementary Numerical Analysis*, McGraw-Hill Book Co., Inc., New York (1965).
49. C. E. Forsythe and C. B. Mohr, *Computer Solution of Linear Algebraic Systems*, Prentice-Hall, Inc., Englewood Cliffs, New Jersey (1967).
50. L. J. Koch, et al., *Hazards Summary Report Experimental Breeder Reactor II (EBR-II)*, ANL-5719 (1957).
51. L. J. Habegger and C. Hsu, *Space-dependent Transfer-Function Analysis of Large Nuclear Reactor Power Systems*, ANL-7788 (Mar 1971).
52. J. H. Seinfeld and L. Lapidus, *Computational Aspects of the Optimal Control of Distributed Parameter Systems*, Chem. Eng. Sci., 23, 1461-1483 (1968).
53. A. P. Sage and S. P. Chaudhuri, *Gradient and Quasi-linearization Computational Techniques for Distributed Parameter Systems*, International Journal of Control, 6(1) 81-98 (1967).
54. D. R. Hahn, *Optimal Control of a Class of Distributed Parameter Process*, Ph.D. Dissertation, Kansas State University (1969). (University of Michigan microfilm, No. 69-21, 126).
55. J. Greenstadt, *On the Relative Efficiencies of Gradient Methods*, Mathematics of Computation, 21, 360-367 (1967).
56. H. O. Hartley, *The Modified Gauss-Newton Method for the Fitting of Nonlinear Regression Functions by Least Squares*, Technometrics, 3(2), 269-280 (1961).
57. M. R. Hestenes and E. Stiefel, *Method of Conjugate Gradients for Solving Linear Systems*, Report 1659, National Bureau of Standards (1952).
58. F. S. Beckman, "The Solution of Linear Equations by the Conjugate Gradient Method," in *Mathematical Methods for Digital Computers*, edited by A. Ralston and H. S. Wilf, John Wiley and Sons, New York (1960).
59. R. Fletcher and C. M. Reeves, *Function Minimization by Conjugate Gradients*, Computer Journal, 7, 149-153 (1964).
60. W. C. Davidon, *Variable Metric Method for Minimization*, ANL-5990 (Rev.) (1959).

61. R. Fletcher and M. J. D. Powell, *A Rapidly Convergent Descent Method for Minimization*, Computer Journal, 6, 163-168 (1963).
62. H. Y. Huang, *Unified Approach to Quadratically Convergent Algorithms for Function Minimization*, J. of Optimization Theory and Applications, 5(6), 405-423 (1970).
63. R. D. Richtmyer and K. W. Morton, *Difference Methods for Initial-Value Problems*, Interscience Publishers, New York (1967).
64. L. Fox, *Numerical Solution of Ordinary and Partial Differential Equations*, Addison-Wesley Publishing Co., Inc., Reading, Mass. (1962).
65. D. U. VonRosenberg, *Methods for the Numerical Solution of Partial Equations*, Americal Elsevier Publishing Co., Inc., New York (1969).
66. F. B. Hildebrand, *Finite-Difference Equations and Simulations*, Prentice-Hall, Inc., Englewood Cliffs, New Jersey (1968).
67. A. R. Mitchell, *Computational Methods in Partial Differential Equations*, John Wiley and Sons, Inc., New York (1969).
68. E. H. Herron and D. U. VonRosenberg, *An Efficient Numerical Method for the Solution of Pure Convective Transport Problems with Split Boundary Conditions*, Chem. Eng. Sci., 21, 337-342 (1966).
69. J. C. Wyngaard and F. W. Schmidt, *A Comparison of Methods for Determining the Transient Response of a Shell-and-Tube Heat Exchanger*, ASME Publication No. 64-WA/HT-20 (1964).
70. J. F. L. M. Brukx, *CSDT Simulation Model for Prediction of IHX Transient Behavior Using S/360 CSMP*, M.S. Thesis, Technological University Delft, Delft, The Netherlands (Dec 1970).
71. W. M. Stacey, *Space-Time Nuclear Reactor Kinetics*, Academic Press, New York (1969).