QUASILINEARIZATION APPLIED TO NONLINEAR BOUNDARY-VALUE PROBLEMS IN OPTIMAL MANAGEMENT SYSTEMS

by

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CHAPTER 1

INTRODUCTION

In industrial management systems, such as inventory and production control, many of the mathematical models are governed by ordindary differential equations with two-point or multipoint boundary-conditions. Usually they appear in nonlinear forms. There is no general method for solving problems of this type neither analytically nor numerically. One of the most frequently used methods to obtain solutions for these problems is the trial-and-error method which is very tedious and inefficient.

The quasilinearization technique which was first developed by Bellman and Kalaba [1], is a powerful tool for solving boundary-value problems. It has been applied by many analysts to many different fields. Kenneth and McGill [2] have used this technique to solve the boundary value problem resulting from the application of the Pontryagin maximum principle. Ramaker, Smith, and Murrill [3] showed that quasilinearization can be used to determine model parameters including a dead time. Schulz [4] used this technique to estimate the parameters of a pulse transfer function. To investigate how this method behaved on a complex engineering problem, Leondes and Paine [5] applied the quasilinearization technique to find the trajectory that minimizes the convective heating in a space vehicle. Lewallen [6] modified the quasilinearization method in order to handle terminal conditions which are general functions of the problem variables rather than specific values of the variables. Lee [7] has given a detailed description of the applications of quasilinearization to parameter estimation problems as well as optimization problems. He also combined quasilinearization with calculus of variations, Pontryagin's maximum principle, invariant imbedding, and dynamic programming.

Recently, Shah [8] applied the quasilinearization technique to an industrial management system which deals with the advertisement, inventory, and production of a particular chemical product. In this work, the technique will be used for the simultaneous optimization of the control and system parameters of production planning and inventory control systems.

1-1 QUASILINEARIZATION

The quasilinearization technique is essentially a generalized Newton-Raphson formula for functional equations. In this technique, the nonlinear differential equations are solved recursively by a series of linear differential equations. The linear equation is obtained by applying the Taylor's series expansion with the second and higher order terms omitted.

These linearized differential equations can be solved easily on the modern digital computer with the use of the superposition principle [9].

The main advantage of this technique is that if the procedure converges, it converges quadratically to the solution of the original equation.

1-2 OPTIMIZATION PROBLEM WITH PARAMETERS

The development of a model for a given system has become important in all fields of engineering. The forms of the differential equations describing various systems often are fairly well documented; however, values of the parameters are usually specific for each system. These parameters generally cannot be measured directly but must be determined from experimental input-output records. Thus, parameter estimation is actually a combination of experimental work with mathematical analysis. Usually an effective mathematical technique can often reduce the requirements for the experimental work.

The parameter estimation problem can be considered as a boundary-value problem and thus can be solved computationally by the use of the quasilinearization technique.

In this thesis, quasilinearization is used to determine the optimal control variables and the optimal values of the parameters in the differential equations which govern industrial management systems.

CHAPTER 2

CALCULUS OF VARIATIONS WITH UNKNOWN PARAMETERS

2-1 INTRODUCTION

The idea of calculus of variations was developed as far back as the 18th century. Later, it was further developed by Bliss [10], Bolza [11], Constantin [12] and many other mathematicians. The calculus of variations is a mathematical concept which may best be described as a general theory of extreme values.

The term "unknown parameters" used here, is considered as a set of constant variables which appear in a system of differential equations. If these differential equations are the representation of an optimization model, then these unknown parameters must be defined before any action can be taken.

Generally speaking, the estimation of these unknown parameters is difficult. The usual procedure for designing such a model is to choose several parameters, optimize the system under these different choices, and then select the most promising combination. In Lee's paper [13], a new approach for the determination of parameters was proposed. It employs the classical calculus of variations and considers the unknown parameters as additional state variables. After optimizing this new system, these parameters are defined. In the next section, the variational equations which essentially follow Lee's algorithm are outlined.

2-2 VARIATIONAL EQUATIONS

Let us consider an optimization problem with parameters. Find the function

$$u(t)$$

and the set of constant parameters

$$a_1,\ a_2,\ \ldots,\ a_q$$

such that the set of functions

$$x_1(t),\ \ldots,\ x_n(t)$$

governed by the differential equations

$$x_i(t) = f_i(x_1,\ \ldots,\ x_n,\ a_1,\ \ldots,\ a_q,\ t,\ u) \qquad i = 1,\ 2,\ \ldots,\ n \tag{2-1}$$

and the end conditions

$$h_j(t_0,\ x_1(t_0),\ \ldots,\ x_n(t_0),\ t_f,\ x_1(t_f),\ \ldots,\ x_n(t_f),\ a_1,\ \ldots,\ a_q) \qquad j = 1,\ \ldots,\ p \le 2n + 2 \tag{2-2}$$

which minimize a function of the form

$$J = g(t_0,\ x_1(t_0),\ \ldots,\ x_n(t_0),\ t_f,\ x_1(t_f),\ \ldots,\ x_n(t_f),\ a_1,\ \ldots,\ a_q) + \int_{t_0}^{t_f} f_0(x_1(t),\ \ldots,\ x_n(t),\ a_1,\ \ldots,\ a_q,\ u,\ t)dt \tag{2-3}$$

where $\dot{x}$ represents $\frac{dx}{dt}$.

The variables $x_1(t)$, ..., $x_n(t)$ are the state variables and the variable $u(t)$ is the control variable. The problem formulated above is known as the problem of Bolza except for the presence of the unknown constant parameters. However, this difference can be eliminated if we consider the constant parameters as functions of t and treat them as state variables. Let

$$\frac{da_k(t)}{dt} = 0, \qquad k = 1, 2, \ldots, q \tag{2-4}$$

and let $x_{n+1}(t)$, $x_{n+2}(t)$, ..., $x_{n+q}(t)$ denote $a_1(t)$, $a_2(t)$, ..., $a_q(t)$ respectively.

Now let us introduce the set of Lagrange multipliers

$$\lambda_i(t), \qquad i = 1, 2, \ldots, n, \ldots, (n+q)$$

and the set of constant multipliers:

$$v_j \quad , \qquad j = 1, 2, \ldots, p$$

Define the function

$$F(t, \bar{x}, \bar{\dot{x}}, u, \bar{\lambda}) = \sum_{i=1}^{n=q} \lambda_i(\dot{x}_i - f_i(t, u, x)) + f_o(x, u, t) \tag{2-5}$$

$$G(t_o, \bar{x}(t_o), t_f, \bar{x}(t_f)) = g(t_o, \bar{x}(t_o), t_f, \bar{x}(t_f)) + \sum_{j=1}^{p} v_j \, h_j(t_o, \bar{x}(t_o), t_f, \bar{x}(t_f)) \tag{2-6}$$

where $\bar{x}$, $\bar{\dot{x}}$, and $\bar{\lambda}$ represent $x_1, \ldots, x_{n+q}$; $\dot{x}_1, \ldots, \dot{x}_{n+q}$; and $_1, \ldots, \lambda_{n+q}$, respectively.

The Euler-Lagrange equations are

$$\frac{d}{dt}\frac{\partial F}{\partial x_i} - \frac{\partial F}{\partial x_i} = 0\,, \qquad i = 1, \ldots, n+q \tag{2-7}$$

$$\frac{\partial F}{\partial u} = 0\,. \tag{2-8}$$

The equation

$$\left[\left(F - \sum_{1}^{n+q} x_i \frac{\partial F}{\partial x_i}\right)dt + \sum_{1}^{n+q} \frac{\partial F}{\partial x_i}\,dx_i\right]\Bigg|_{t_f} - \left[\left(F - \sum_{1}^{n+q} x_i \frac{\partial F}{\partial x_i}\right)dt + \sum_{1}^{n+q} \frac{\partial F}{\partial x_i}\,dx_i\right]\Bigg|_{t_o} + dG = 0 \tag{2-9}$$

must be satisfied at t_o and t_f for any choice of $dx(t_o)$, $dx(t_f)$, dt_o, and dt_f. This simply means that all their corresponding coefficients must equal to zero.

$$\left[-F + \sum_{1}^{n+q} x_i \frac{\partial F}{\partial x_i}\right]\Bigg|_{t_o} + \frac{\partial G}{\partial t}\Bigg|_{t_o} = 0$$

$$\left[F - \sum_{1}^{n+q} x_i \frac{\partial F}{\partial x_i}\right]\Bigg|_{t_f} + \frac{\partial G}{\partial t}\Bigg|_{t_f} = 0 \tag{2-10}$$

$$\frac{\partial G}{\partial x_i}\Bigg|_{t_o} - \frac{\partial F}{\partial x_i}\Bigg|_{t_o} = 0$$

$$\frac{\partial G}{\partial x_i}\Bigg|_{t_f} + \frac{\partial F}{\partial x_i}\Bigg|_{t_f} = 0 \tag{2-11}$$

Equation (2-9) or equations (2-10) and (2-11) are known as transversality condition.

By solving equations (1), (7), and (8), the stationary point of the original problem can be obtained. Notice that originally we have (n+q) equations with (n+q) unknown x's plus one unknown u. After reformulating the original problem, we have 2(n+q) + 1 equations with (n+q) unknown x's, (n+q) unknown λ's and one unknown u, there is a total of 2(n+q)+1 unknowns. By the use of transversality condition and plus the original given conditions we have exact 2(n+q) conditions for the 2(n+q) differential equations. These conditions are not all given at one point. The above system will always be a boundary-value problem.

CHAPTER 3

QUASILINEARIZATION AND BOUNDARY-VALUE PROBLEMS

3-1 INTRODUCTION

The quasilinearization technique, as mentioned before, is essentially a generalized Newton-Raphson method for functional equations. However, the quasilinearization technique is able to obtain the functional solutions while the Newton-Raphson Method is generally used for obtaining fixed values or roots. Therefore, both the computational and theoretical aspects are much more complicated.

This technique not only linearizes the nonlinear equation, it also provides a sequence of functions which converge rapidly to the true solution of the original nonlinear equation.

In earlier times, the preferred procedure for solving the nonlinear boundary-value problem was to simplify so as to obtain linear functional equations. Another attempt has been made is to transform all computational equations to initial value problems for ordinary differential equations, either linear or nonlinear. The theory of dynamic programming and invariant imbedding achieve this in a number of ways through the introduction of new state variable and the use of semigroup properties in space, time, and structure. Quasilinearization achieves this objective by combining linear approximation techniques with the capabilities of the digital computer in various adroit fashions. The approximations are carefully constructed to yield rapid convergence, and monotonicity as well, in many cases.

This chapter is concerned with the procedure of solving a two-point nonlinear boundary-value problem. Since most of the work deals with the numerical solution, a brief description of the initial-value problem and its solution will be given in section 2. The boundary-value problem is also included in this section. The superposition principle is explained in section 3. At last the quasilinearization technique will be explained.

3-2 INITIAL-VALUE AND BOUNDARY-VALUE PROBLEM

Initial-value problems are those in which all conditions are given at one point. This particular point can be the initial or final point of the entire interval.

In numerical approaches, the values of the dependent variables are calculated at discrete values of the independent variable. In other words, the dependent variables are calculated step by step with a very small division of the independent variable as the step size. There are various numerical integration methods available for obtaining the solution. For detailed description of these methods, readers are referred to Ralston [15] and Tompkin [16].

All the numerical integration methods require the complete set of initial conditions. Knowing the initial values of all the variables, then it is able to calculate values of the variables at the next grid point. Thus, only the initial-value problem is suited for these integration methods. Boundary-value problems are those in which the necessary conditions are not given at one point

The numerical integration method is useless unless all the necessary conditions are given at one point either at the initial or at the final point. In order to find the solution of a boundary-value problem, some missing conditions have to be assumed. But when faced with a nonlinear or very complex problem, it is very difficult to find the solution in this fashion. This situation is generally known as the boundary value difficulty.

3-3 SUPERPOSITION PRINCIPLE

The superposition principle states the additive property of the solution of a linear ordinary differential equation. To explain this property, one may consider a system of linear differential equations.

$$\frac{dx_i}{dt} = a_0 + \sum_{n=1}^{n} a_i \, x_i \qquad i = 1, 2, \ldots, n \tag{3-1}$$

with boundary conditions

$$x_k(t_0) = x_k^0 \qquad k = 1, \ldots, s < n \tag{3-2}$$

and

$$x_r(t_f) = x_r^1 \qquad r = s+1, \ldots, n \tag{3-3}$$

The general solution of Equation (3-1), stated by the superposition principle can be written as

$$x_i(t) = x_{p,i}(t) + \sum_{j=1}^{n} A_j \, x_{h,i,j}(t)$$

$$i = 1,\ 2,\ \ldots,\ n \tag{3-4}$$

Where $x_{p,i}(t)$ stands for the particular solution of $x_i(t)$ which can be integrated by using any arbitrarily assumed initial conditions for Eq. (3-1). Where $x_{h,i,j}$ stands for the homogeneous solution of the variable x_i. The subscript j stands for the jth set of homogeneous solution of x_i. The homogeneous solution is obtained by integrating Eq. (3-1) in the homogeneous form which is obtained by setting all the constant terms equal to zero. The homogeneous form of Eq. (3-1) can be written as

$$\frac{dx_i}{dt} = \sum_{i=1}^{n} a_i \, x_i \qquad i = 1,\ \ldots,\ n \tag{3-5}$$

In order to solve Eq. (3-5) for the homogeneous solutions, any n sets of initial conditions can be used provided they are non-trivial.

The expression A_j is the integration constant, which can be obtained by substituting the boundary conditions (3-2) and (3-3) into Eq. (3-4). Once all the A_j's are known, the solution for $x_i(t)$ is completely known at every grid point.

If appropriate initial conditions are chosen for the particular and homogeneous solutions which satisfy the given boundary conditions, then the number of the required sets of homogeneous solutions can be reduced.

It is important to note that the particular and homogeneous solutions can be obtained numerically. The superposition principle actually transforms the above linear boundary-value problem into a linear initial-value problem.

For more detailed discussion about the superposition principle and the reduction of homogeneous sets, the reader is referred to Ince [9] and Lee [7].

3-4 QUASILINEARIZATION

To explain how the quasilinearization technique works, the generalized Newton-Raphson method for differential equations will be discussed first. Consider the nonlinear differential equation

$$\frac{dx}{dt} = f(x(t),\ t) \quad \text{and} \quad x(t_0) = c \tag{3-8}$$

The function f can be expanded around the function $x_0(t)$ by the use of the Taylor series

$$f(x(t),\ t) = f(x_0(t),\ t) + (x(t) - x_0(t))f_{x_0}(x_0(t),\ t) \tag{3-9}$$

with the second - and higher-order terms omitted. The expression f_{x_0} represents partial differentiation of the function f with respect to x_0. Combining Eqs. (3-8) and (3-9) and rearranging terms, the following equation is obtained:

$$\frac{dx}{dt} = f_{x_o}(x_o(t), t)x(t) + f(x_o(t), t) - f_{x_o}(x_o(t), t)x_o(t) \tag{3-10}$$

Notice that $x_o(t)$ are known functions of t. Eq. (3-10) is a linear differential equation with variable coefficients. This is the algorithm which quasilinearization employes to linearize nonlinear equations.

Now let us consider a general nonlinear system :

$$\frac{d\overline{X}}{dt} = \overline{f}(\overline{X}, t) \tag{3-11}$$

where $\overline{X}$ and $\overline{f}$ are m-dimensional vectors with components x_1, x_2, ..., x_m and f_1, f_2, ..., f_m respectively.

If we choose a set of initial approximations for x_1, x_2, ..., x_m and denote them as $x_{1,0}$, $x_{2,0}$, ..., $x_{m,0}$. Eq. (3-11) can be linearized by the use of the following vector equation

$$\frac{d\overline{X}}{dt} = \overline{f}(\overline{X}, t) = \overline{f}(\overline{X}_o, t) + J(\overline{X}_o)(\overline{X} - \overline{X}_o) \tag{3-12}$$

where $\overline{X}_o$ is an m-dimensional vector with components $x_{1,0}$, $x_{2,0}$, ..., $x_{m,0}$. The Jacobi matrix $J(\overline{X}_o)$ is defined by

$$J(\overline{X}_0) = \begin{bmatrix} \frac{\partial f_1}{\partial x_{1,0}} & \frac{\partial f_1}{\partial x_{2,0}} & \cdots & \frac{\partial f_1}{\partial x_{m,0}} \\ \frac{\partial f_2}{\partial x_{1,0}} & \frac{\partial f_2}{\partial x_{2,0}} & \cdots & \frac{\partial f_2}{\partial x_{m,0}} \\ & & \vdots & \\ \frac{\partial f_m}{\partial x_{1,0}} & \frac{\partial f_m}{\partial x_{2,0}} & \cdots & \frac{\partial f_m}{\partial x_{m,0}} \end{bmatrix} \tag{3-13}$$

Assume the boundary conditions for Eq. (3-11) are

$$\begin{aligned} x_i(t_0) &= x_i^0 \, ; \qquad i = 1,\ 2,\ \ldots,\ p < m \\ x_j(t_f) &= x_j^1 \, ; \qquad j = p+1,\ \ldots,\ m \end{aligned} \tag{3-14}$$

By the use of superposition principle, linearized Eq. (3-12) can be solved easily with known $\overline{X}_0$ functions and the conditions given above. The solution we get is an improved set of solutions. Let this improved solution be $\overline{X}_1$ which can be used as a new initial approximation. A new improved solution $\overline{X}_2$ can now be obtained. If this procedure is continued, the following recurrence relation is obtained:

$$\frac{d\overline{X}_{n+1}}{dt} = \overline{f}(\overline{X}_n,\ t) + J(\overline{X}_n)(\overline{X}_{n+1} - \overline{X}_n) \tag{3-15}$$

where $J(\overline{X}_n)$ is the Jacobi matrix defined as

$$J(X_n) = \begin{bmatrix} \frac{\partial f_1}{\partial x_{1,n}} & \frac{\partial f_1}{\partial x_{2,n}} & \cdots & \frac{\partial f_1}{\partial x_{m,n}} \\ \frac{\partial f_2}{\partial x_{1,n}} & \frac{\partial f_2}{\partial x_{2,n}} & \cdots & \frac{\partial f_2}{\partial x_{m,n}} \\ & & \vdots & \\ \frac{\partial f_m}{\partial x_{1,n}} & \frac{\partial f_m}{\partial x_{2,n}} & \cdots & \frac{\partial f_m}{\partial x_{m,n}} \end{bmatrix} \tag{3-16}$$

From the computational standpoint, quasilinearization has two important properties, namely monotone convergence and quadratic convergence. The monotone convergence property depends on the property of the function $\overline{f}$.

This technique also has its difficulties. One main difficulty is caused by the use of superposition principle. When the superposition principle is applied, a set of algebraic equations must be solved when finding the integration constants. Thus ill-conditioned equations can make the superposition principle useless. Another main difficulty is the convergence problem. If the initial approximation is too far from the true solution, the problem will not converge.

For more detailed discussion, the reader is referred to Lee [7].

CHAPTER 4

OPTIMAL PRODUCTION PLANNING PROBLEM WITH UNKNOWN PARAMETERS

In this chapter, a management system with unknown parameters will be solved. It deals with the advertisement, inventory, and production planning of a particular chemical product. This model has six state variables, one control variable and two parameters. Most of these variables and parameters appear nonlinearly in the system equations. Usually, a large dimensional and nonlinear model can seldom be solved analytically. Thus, an efficient numerical method has to be used to solve this model. Throughout this chapter, quasilinearization is used to find the optimal solution of this model combined with the calculus of variations

4-1 DEVELOPMENT OF THE MODEL

A firm produces a chemical product and sells it in a market which can absorb a certain amount of the product per unit of time. If the firm advertises, the rate of sales will increase at a rate proportional to the rate of advertising. The relation between advertisement and sales which may expressed using the diffussion model developed by Teichroew [17] is discussed first as follows.

Consider a group of people in which only certain member possesses a particular piece of information. Suppose that the total number of persons in the group remains constant and that the diffusion of information only occurs through personal contact. Each person in the group has the same "contact coefficient" in any unit of time; this coefficient is a fixed pure number. In a contact, the contactee receives the information only if he does not already have it; otherwise the contact is a waste.

Let $M(0)$ = number of informed people in the group at time 0.

N = total number of people in the group.

C_c = contact coefficient; the number of contacts made by one informed person per unit time.

$M(t)$ = number of informed persons in the group at time t.

$\frac{M(t)}{N}$ = proportion of informed persons in the group at time t.

$1 - \frac{M(t)}{N}$ = proportion of uninformed persons in the group at time t.

$C_c M(t)dt$ = contacts made during a time interval dt.

The increase in the total number of informed people during a short interval of time dt is obtained by multiplying the number of contacts by the proportion of uninformed persons, since only contacts with uninformed group members leads to an increase in informed members:

$$dM(t) = C_c M(t)\, dt\, (1 - \frac{M(t)}{N}) \tag{4-1}$$

This is the differential equation

$$\frac{dM(t)}{dt} = C_c M(t)(1 - M(t)/N) \tag{4-2}$$

Suppose the firm can increase the number of contacts by advertising. This simply means that advertisement may increase the contact coefficient. Let A(t) represent the increase of contact by advertisement at time t. Thus,

$$\frac{dM(t)}{dt} = (C_c + A(t))\, M(t)\, (1 - M(t)/N) \tag{4-3}$$

If each imformed person buys C_q units of the firm's product and if S(t) represents the sale at time t, then

$$S(t) = C_q M(t) \tag{4-4}$$

Let $C_q = 1$, and substitute for M(t) in Eq. (4-3),

$$\frac{d\,S(t)}{dt} = S(t)\, (C_c + A(t))\, (1 - \frac{S(t)}{N}) \tag{4-5}$$

The rate of change of the firm's inventory, I(t), is given by

$$\frac{d\ I(t)}{dt} = p(t) - S(t) \tag{4-6}$$

where $p(t) =$ production rate at time t.

The manufacturing process of the product is shown schematically in Fig. A. There are two chemical reactors in which the following reactions take place

$$A \longrightarrow B \longrightarrow C$$

Both these reactions are first order. The component B is the desired product and C is a waste product. Assume that A and C have unlimited market at fixed price and B is the new product described above. Furthermore, to protect against fluctuations in demand, an inventory will be assumed for B. Of course, there is a cost associated with the inventory.

Let x_1, y_1 and x_2, y_2 represent the concentration of A and B in reactor 1 and 2 respectively.

Let

V_i = volume of chemical reactor i ; i=1, 2 ,

q = flow rate ,

K_{ai} = reaction rate constant of the first reaction in reactor i ,

K_{bi} = reaction rate constant of the second reaction in reactor i ,

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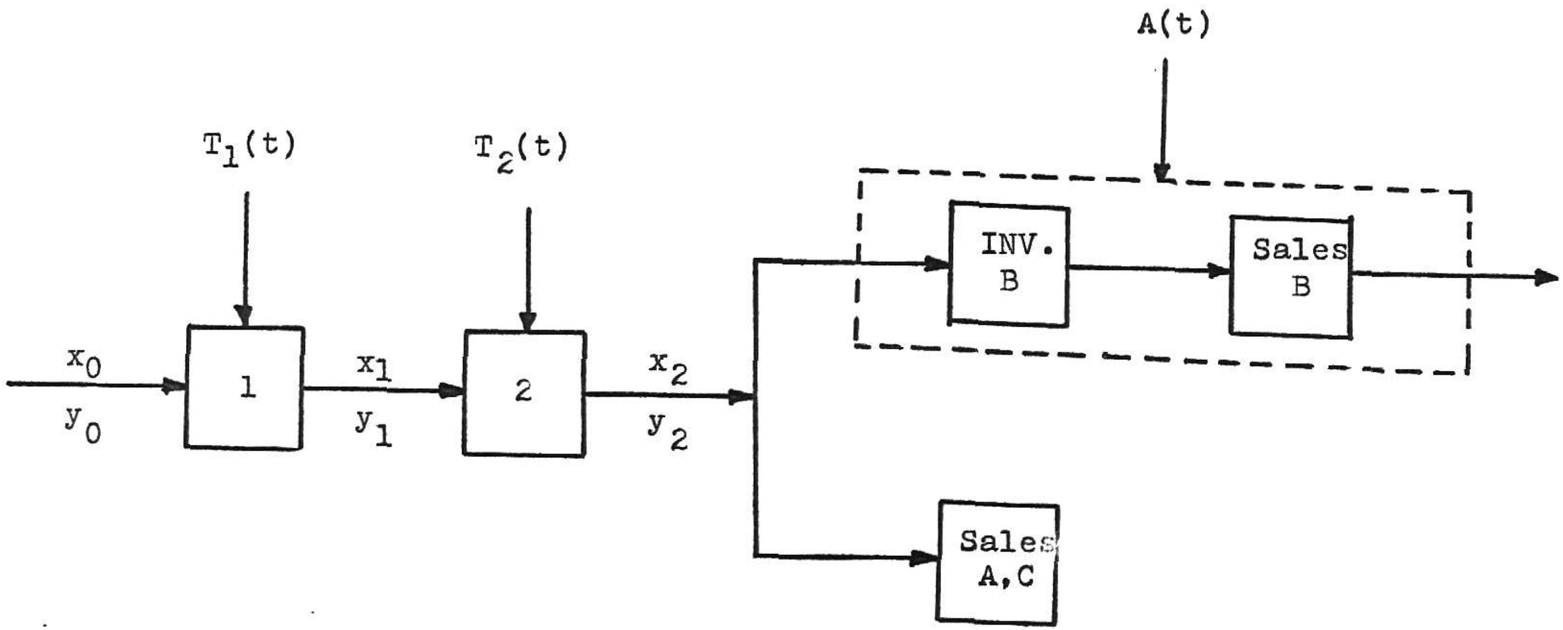

Fig. A. Advertisement and Production Model

G_a, G_b = frequency constants of the first and second reactions, respectively,

E_a, E_b = activation energies of the first and second reactions, respectively,

R = gas constant,

T_i = temperature in reactor i (4-8)

The kinetics of the reactions for x_1, in reactor 1 can now be written as

$$q\ x_0 = q\ x_1 + V_1\ K_{a1}\ x_1 \tag{4-9}$$

or

$$q(x_0 - x_1) - V_1\ K_{a1}\ x_1 = 0 \tag{4-10}$$

at steady state. Under unsteady state situations, we have

$$V_1 \frac{dx_1}{dt} = q(x_0 - x_1) - V_1\ K_{a1}\ x_1 \tag{4-11}$$

similarly, For y_1 in reactor 1, we have

$$q\ y_0 = q\ y_1 + V_1\ K_{b1} y_1 - V_1\ K_{a1}\ x_1 \tag{4-12}$$

or

$$q(y_0 - y_1) - V_1\ K_{b1}\ y_1 + V_1\ K_{a1}\ x_1 = 0 \tag{4-13}$$

at steady state. Under unsteady state, we have

$$V_1 \frac{dy_1}{dt} = q(y_0 - y_1) - V_1 K_{b1} y_1 + V_1 K_{a1} x_1 \qquad (4\text{-}14)$$

with similar treatment, the kinetics of the reactions in the second reactor can be written as

$$V_2 \frac{dx_2}{dt} = q(x_1 - x_2) - V_1 K_{a2} x_1 \qquad (4\text{-}15)$$

and

$$V_2 \frac{dy_2}{dt} = q(y_1 - y_2) - V_1 K_{b1} y_1 + V_2 K_{a2} x_2 \qquad (4\text{-}16)$$

The reaction rate constants are defined as

$$\begin{aligned} K_{a1} &= G_a \exp(-\frac{E_a}{RT_1}) \quad , \quad K_{b1} = G_b \exp(-\frac{E_b}{RT_1}) \\ K_{a2} &= G_a \exp(-\frac{E_a}{RT_2}) \quad , \quad K_{b2} = G_b \exp(-\frac{E_b}{RT_2}) \end{aligned} \qquad (4\text{-}17)$$

Since only B product has inventory, the production rate $p(t)$ in Eq. (4-6) is equal to

$$p(t) = q\, y_2(t) \qquad (4\text{-}18)$$

Substitute this into Eq. (6), we have

$$\frac{d\ I(t)}{dt} = q\ y_2(t) - S(t) \tag{4-19}$$

Now, this model is completely defined by Equations (5), (11), (14), (15), (16), and (19). There are six state variables, x_1, y_1, x_2, y_2, I, and S; and three control variables, T_1, T_2, and A.

In this particular chemical reaction the temperature in the reactors plays a very important roll. In Shah's thesis [8], he solved this problem by obtaining optimal control temperature profile which is a function of t. The control of temperature usually is difficult. In this development, the temperature will be considered as a constant parameter, whose optimal value is to be decided.

The unknown parameters can be treated as additional state variables, and since these state variables are constant with respect to time, they can be described by the differential equations

$$\frac{dT_1}{dt} = 0 \tag{4-20}$$

$$\frac{dT_2}{dt} = 0 \tag{4-21}$$

Equations (5), (11), (14), (15), (16), (19), (20) and (21) now govern the system. Instead of having three control variables, we have one control variable and two parameters.

The objective of the firm for this production is

$$\text{profit} = \int_{t_o}^{t_f} \Big[\text{revenue of B} + \text{revenue of A} + \text{revenue of C} - \begin{matrix}\text{inventory}\\ \text{cost}\end{matrix} - \begin{matrix}\text{advertisement}\\ \text{cost}\end{matrix} - \begin{matrix}\text{manufacturing}\\ \text{cost}\end{matrix}\Big]\, dt \tag{4-22}$$

If we define

C_1 = profit per unit sale of B ,

C_2 = profit per unit sale of A,

C_3 = profit per unit sale of C,

C_I = inventory cost per unit product of B,

C_A = advertisement cost,

C_T = cost of changing per degree of temperature,

I_m = ideal quantity of inventory,

T_{1m} = the temperature of raw material,

then, the profit function can be expressed mathematically as

$$J = \int_{t_o}^{t_f} [C_1 \cancel{q} S + C_2 q x_2 + C_3 q(1 - x_2 - y_2) - C_I(I_m - I)^2 - C_A A^2 S^2]dt - C_T[(T_{1m} - T_1(0))^2 + (T_1(0) - T_2(0))^2] \tag{4-23}$$

The management in this particular system is concerned with the problem of selecting one control variable and two parameters such that the above function J is maximized.

4-2 DEFINITION OF THE PROBLEM

Maximize the function

$$J = \int_{t_o}^{t_f} [C_1 C_q S + C_2 q x_2 + C_3 q(1 - x_2 - y_2) - C_I(I_m - I)^2 - C_A A\,S]dt - C_T\left\{[T_{1m} - T_1(0)]^2 + [T_1(0) - T_2(0)]^2\right\} \tag{4-24}$$

subject to the constraints of

$$V_1 \frac{dx_1}{dt} = q(x_0 - x_1) - V_1 K_{a1} x_1 \tag{4-25}$$

$$V_1 \frac{dy_1}{dt} = q(y_0 - y_1) - V_1 K_{b1} y_1 + V_1 K_{a1} x_1 \tag{4-26}$$

$$V_2 \frac{dx_2}{dt} = q(x_1 - x_2) - V_2 K_{a2} x_2 \tag{4-27}$$

$$V_2 \frac{dy_2}{dt} = q(y_1 - y_2) - V_2 K_{b2} y_2 + V_2 K_{a2} x_2 \tag{4-28}$$

$$\frac{dI}{dt} = q\, y_2 - S \tag{4-29}$$

$$\frac{dS}{dt} = S(C_c + A)(1 - \frac{S}{N}) \tag{4-30}$$

$$\frac{dT_1}{dt} = 0 \tag{4-31}$$

$$\frac{dT_2}{dt} = 0 \tag{4-32}$$

with boundary conditions

$$\begin{array}{lll} x_1(t_0) = x_1^0 & y_1(t_0) = y_1^0 & \\ x_2(t_0) = x_2^0 & y_2(t_0) = y_2^0 & I(t_f) = I^1 \\ I\ (t_0) = I^0 & S\ (t_0) = S^0 & \end{array} \tag{4-33}$$

given for the above differential equations.

4-3 FORMULATION OF THE PROBLEM

In this problem, we wish to find the optimal value of state variables, control variable and parameters. This problem is the Bolza's problem, which is in the same form as we have discussed in Chapter 2. This problem will be solved by the use of calculus of variations with the help of quasilinearization.

Equations (25) through (32) can be rewritten as

$$\dot{x}_1 - \frac{q}{V_1}(x_0 - x_1) + G_a\, e^{-\frac{E_a}{RT_1}} x_1 = 0 \tag{4-34}$$

$$\dot{y}_1 - \frac{q}{V_1}(y_0 - y_1) + G_b e^{-\frac{E_b}{RT_1}} y_1 - G_a e^{-\frac{E_a}{RT_1}} x_1 = 0 \tag{4-35}$$

$$\dot{x}_2 - \frac{q}{V_2}(x_1 - x_2) + G_a e^{-\frac{E_a}{RT_2}} x_2 = 0 \tag{4-36}$$

$$\dot{y}_2 - \frac{q}{V_2}(y_1 - y_2) + G_b e^{-\frac{E_b}{RT_2}} y_2 - G_a e^{-\frac{E_a}{RT_2}} x_2 = 0 \tag{4-37}$$

$$\dot{I} - q\, y_2 + S = 0 \tag{4-38}$$

$$\dot{S} - (C_c S + AS)(1 - \frac{S}{N}) = 0 \tag{4-39}$$

where $\dot{x}_1$ stands for $\frac{dx_1}{dt}$.

Introduce Lagrange multipliers, λ_i, $i = 1, 2, \ldots, 8$; and constant multipliers θ_j, $j = 1, 2, \ldots, 7$, and define the following functions

$$\begin{aligned} F = \Big[& \lambda_1(\dot{x}_1 - \frac{q}{V_1}(x_0 - x_1) + G_a e^{-\frac{E_a}{RT_1}} x_1) \\ & + \lambda_2(\dot{y}_1 - \frac{q}{V_1}(y_0 - y_1) + G_b e^{-\frac{E_b}{RT_1}} y_1 - G_a e^{-\frac{E_a}{RT_1}} x_1) \\ & + \lambda_3(\dot{x}_2 - \frac{q}{V_2}(x_1 - x_2) + G_a e^{-\frac{E_a}{RT_2}} x_2) \\ & + \lambda_4(\dot{y}_2 - \frac{q}{V_2}(y_1 - y_2) + G_b e^{-\frac{E_b}{RT_2}} y_2 - G_a e^{-\frac{E_a}{RT_2}} x_2) \\ & + \lambda_5(\dot{I} - q\, y_2 + S) \\ & + \lambda_6(\dot{S} - (C_c S + AS)(1 - \frac{S}{N})) \\ & + \lambda_7(\dot{T}_1) + \lambda_8(\dot{T}_2) + C_1 C_q S + C_2 q\, x_2 \\ & + C_3 q(1 - x_2 - y_2) - C_I(I_m - I)^2 - C_A A^2 S^2 \Big] \end{aligned} \tag{4-40}$$

and

$$G = [\theta_1(x_1(0) - x_1^0) + \theta_2(y_1(0) - y_1^0) + \theta_3(x_2(0) - x_2^0)$$
$$+ \theta_4(y_2(0) - y_2^0) + \theta_5(I(0) - I^0) + \theta_6(I(t_f) - I^1)$$
$$+ \theta_7(S(0) - S^0) - C_T[(T_{1m} - T_1(0))^2$$
$$+ (T_1(0) - T_2(0))^2] \qquad (4\text{-}41)$$

The Euler-Lagrange equations (2-7) and (2-8),

$$\frac{d}{dt}\frac{\partial F}{\partial x_i} - \frac{\partial F}{\partial x_i} = 0$$

$$\frac{\partial F}{\partial u} = 0$$

can now be applied to equation (40). The following Lagrange equations are obtained:

$$\frac{d\lambda_1}{dt} = q(\frac{\lambda_1}{V_1} - \frac{\lambda_3}{V_2}) + (\lambda_1 - \lambda_2)G_a e^{-\frac{E_a}{RT_1}} \qquad (4\text{-}42)$$

$$\frac{d\lambda_2}{dt} = q(\frac{\lambda_2}{V_1} - \frac{\lambda_4}{V_2}) + \lambda_2 G_b e^{-\frac{E_b}{RT_1}} \qquad (4\text{-}43)$$

$$\frac{d\lambda_3}{dt} = q\frac{\lambda_3}{V_2} + (\lambda_3 - \lambda_4)G_a e^{-\frac{E_a}{RT_2}} + q(C_2 - C_3) \qquad (4\text{-}44)$$

$$\frac{d\lambda_4}{dt} = q\frac{\lambda_4}{V_2} + \lambda_4 G_b e^{-\frac{E_b}{RT_2}} - q(C_3 + \lambda_5) \qquad (4\text{-}45)$$

$$\frac{d\lambda_5}{dt} = 2\,C_I\,I_m - 2C_I\,I \qquad (4\text{-}46)$$

$$\frac{d\lambda_6}{dt} = C_1C_q + \lambda_5 - C_c\lambda_6 - A\lambda_6 + \frac{2C_cS\lambda_6}{N}$$

$$+ \frac{2AS\lambda_6}{N} - 2\,C_A\,A^2\,S \tag{4-47}$$

$$\frac{d\lambda_7}{dt} = x_1G_ae^{-\frac{E_a}{RT_1}}\left(\frac{E_a}{RT_1^{\,2}}\right)(\lambda_1 - \lambda_2) + \lambda_2y_1G_be^{-\frac{E_b}{RT_1}}\left(\frac{E_b}{RT_1^{\,2}}\right) \tag{4-48}$$

$$\frac{d\lambda_8}{dt} = x_2G_ae^{-\frac{E_a}{RT_2}}\left(\frac{E_a}{RT_2^{\,2}}\right)(\lambda_3 - \lambda_4)$$

$$+ \lambda_4y_2G_be^{-\frac{E_b}{RT_2}}\left(\frac{E_b}{RT_2^{\,2}}\right) \tag{4-49}$$

Applying Eq. (2-8), $\frac{\partial F}{\partial u} = 0$, we get

$$A = \frac{\lambda_6}{2C_A}\left[\frac{1}{N} - \frac{1}{S}\right] \tag{4-50}$$

Since Eq. (50) gives explicit expression of the control variable A, thus A can be eliminated in all the performance equations. As results, Eq. (30) and (47) become:

$$\frac{dS}{dt} = C_cS - \frac{C_cS^2}{N} + \frac{S\lambda_6}{C_AN} - \frac{\lambda_6}{2C_A} - \frac{S^2\lambda_6}{2C_AN^2} \tag{4-51}$$

$$\frac{d\lambda_6}{dt} = C_1C_q + \lambda_5 - C_c\lambda_6 - \frac{\lambda_6^2}{2C_AN} + \frac{2C_cS\lambda_6}{N} + \frac{S\lambda_6^{\,2}}{2C_AN^2} \tag{4-52}$$

Now the sixteen equations, Eqs. (25), (26), (27), (28), (29), (31), (32), (42), (43), (44), (45), (46), (48), (49), (51) and

(52) represent the system. We have only 7 boundary conditions given by Eq. (33). The additional 9 boundary conditions can be obtained by applying the transversality condition, Eq. (2-10) and (2-11)

At $t = t_0$, apply

$$\frac{\partial G}{\partial y_i} - \frac{\partial F}{\partial \dot{y}_i} = 0$$

ie,

$$\frac{\partial G}{\partial T_1(0)} - \frac{\partial F}{\partial \dot{T}_1(0)} = 0 \tag{4-53}$$

and

$$\frac{\partial G}{\partial T_2(0)} - \frac{\partial F}{\partial T_2(0)} = 0 \tag{4-54}$$

The results of Eq. (53) and (54) are two initial conditions:

$$2C_T \left[T_{1m} - T_1(0)\right] - 2\ C_T \left[T_1(0) - T_2(0)\right] = \lambda_7(0)$$

$$2\ C_T \left[T_1(0) - T_1(0)\right] = \lambda_8(0) \tag{4-55}$$

At $t = t_f$, apply Eq. (2-11), the results are 7 final conditions :

$$\lambda_1(t_f) = 0$$

$$\lambda_2(t_f) = 0$$

$$\lambda_3(t_f) = 0$$

$$\lambda_4(t_f) = 0$$

$$\lambda_6(t_f) = 0$$

$$\lambda_7(t_f) = 0$$

$$\lambda_8(t_f) = 0 \tag{4-56}$$

Eq. (55) and (56) give a total of 9 conditions. The whole system is a two-point boundary-value problem.

Assume the case that the final inventory is not given, all we need to do is adding one more condition to Eq. (56). Namely

$$\lambda_5(t_f) = 0 \tag{4-57}$$

The resulting system is still a two-point boundary-value problem.

4-4 QUASILINEARIZATION

Since most of the equations are nonlinear, we are going to linearize these equations using the same procedure described in Chapter 3. Let the vector $\overline{Z}$ represent the state variables

$$\overline{Z} = (x_1, y_1, x_2, y_2, I, S, T_1, T_2, \lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6, \lambda_7, \lambda_8)$$

and let the vector function $\overline{f}$ denote the corresponding differential equations. The original nonlinear system can be represented as

$$\frac{d\overline{Z}}{dt} = \overline{f}(\overline{Z}, t) \tag{4-58}$$

After linearization, the recurrence relations are

$$\frac{d\overline{Z}_{n+1}}{dt} = f_n(\overline{Z}_n) + J(\overline{Z}_n)\ (\overline{Z}_{n+1} - \overline{Z}_n) \tag{4-59}$$

Where $J(\overline{Z}_n)$ is the Jacobi matrix. For clear understanding, the elements of this matrix are given in below

$$\frac{\partial f_1}{\partial Z_1} = -\frac{q}{V_1} - G_a \exp\left(\frac{-E_a}{RZ_7}\right)$$

$$\frac{\partial f_2}{\partial Z_7} = -G_a Z_1 \frac{E_a}{RZ_7^2} \exp\left(\frac{-E_a}{RZ_7}\right)$$

$$\frac{\partial f_2}{\partial Z_1} = G_a \exp\left(\frac{-E_a}{RZ_7}\right)$$

$$\frac{\partial f_2}{\partial Z_2} = -\frac{q}{V_1} - G_b \exp\left(\frac{-E_b}{RZ_7}\right)$$

$$\frac{\partial f_2}{\partial Z_7} = G_a Z_1 \frac{E_a}{RZ_7^2} \exp\left(\frac{-E_a}{RZ_7}\right) - G_b Z_2 \frac{E_b}{RZ_7^2} \exp\left(\frac{-E_b}{RZ_7}\right)$$

$$\frac{\partial f_3}{\partial z_1} = \frac{q}{V_2}$$

$$\frac{\partial f_3}{\partial Z_3} = -\frac{q}{V_2} - G_a \exp\left(\frac{-E_a}{RZ_8}\right)$$

$$\frac{\partial f_3}{\partial Z_8} = -G_a Z_3 \frac{E_a}{RZ_8^2} \exp\left(\frac{-E_a}{RZ_8}\right)$$

$$\frac{\partial f_4}{\partial Z_2} = \frac{q}{V_2}$$

$$\frac{\partial f_4}{\partial Z_3} = G_a \exp\left(\frac{-E_a}{RZ_8}\right)$$

$$\frac{\partial f_4}{\partial Z_4} = -\frac{q}{V_2} - G_b \exp\left(\frac{-E_b}{RZ_8}\right)$$

$$\frac{\partial f_4}{\partial Z_8} = G_a Z_3 \frac{E_a}{RZ_8^2} \exp\left(\frac{-E_a}{RZ_8}\right) - G_b Z_4 \frac{E_b}{RZ_8^2} \exp\left(\frac{-E_b}{RZ_8}\right)$$

$$\frac{\partial f_5}{\partial Z_4} = q$$

$$\frac{\partial f_5}{\partial Z_6} = -1$$

$$\frac{\partial f_6}{\partial Z_6} = C_c + \frac{Z_{14}}{C_A N} - \frac{2C_c Z_6}{N} - \frac{Z_6 Z_{14}}{C_A N^2}$$

$$\frac{\partial f_6}{\partial Z_{14}} = \frac{Z_6}{C_A N} - \frac{1}{2C_A} - \frac{Z_6^2}{2C_A N^2}$$

$$\frac{\partial f_9}{\partial Z_7} = (Z_9 - Z_{10}) G_a \frac{E_a}{RZ_7^2} \exp\left(\frac{-E_a}{RZ_7}\right)$$

$$\frac{\partial f_9}{\partial Z_9} = \frac{q}{V_1} + G_a \exp\left(\frac{-E_a}{RZ_7}\right)$$

$$\frac{\partial f_9}{\partial Z_{10}} = -G_a \exp\left(\frac{-E_a}{RZ_7}\right)$$

$$\frac{\partial f_9}{\partial Z_{11}} = - \frac{q}{V_2}$$

$$\frac{\partial f_{10}}{\partial Z_7} = Z_{10}\ G_b\ \frac{E_b}{RZ_7^2}\ \exp(\frac{-E_b}{RZ_7})$$

$$\frac{\partial f_{10}}{\partial Z_{10}} = \frac{q}{V_1} + G_b\ \exp(\frac{-E_b}{RZ_7})$$

$$\frac{\partial f_{10}}{\partial Z_{12}} = - \frac{q}{V_2}$$

$$\frac{\partial f_{11}}{\partial Z_8} = (Z_{11} - Z_{12})G_a\ \frac{E_a}{RZ_8^2}\ \exp(\frac{-E_a}{RZ_8})$$

$$\frac{\partial f_{11}}{\partial Z_{11}} = \frac{q}{V_2} + G_a\ \exp(\frac{-E_a}{RZ_8})$$

$$\frac{\partial f_{11}}{\partial Z_{12}} + - G_a\ \exp(\frac{-E_a}{RZ_8})$$

$$\frac{\partial f_{12}}{\partial Z_8} = Z_{12}G_b\ \frac{E_b}{RZ_8^2}\ \exp(\frac{-E_b}{RZ_8})$$

$$\frac{\partial f_{12}}{\partial Z_{12}} = \frac{q}{V_2} + G_b\ \exp(\frac{-E_b}{RZ_8})$$

$$\frac{\partial f_{12}}{\partial Z_{13}} = - q$$

$$\frac{\partial f_{13}}{\partial Z_5} = - 2\ C_I$$

$$\frac{\partial f_{14}}{\partial Z_6} = \frac{2C_c Z_{14}}{N} + \frac{Z_{14}^2}{2C_A N^2}$$

$$\frac{\partial f_{14}}{\partial Z_{13}} = 1$$

$$\frac{\partial f_{14}}{\partial Z_{14}} = - C_c - \frac{Z_{14}}{C_A N} + \frac{2C_c Z_6}{N} + \frac{Z_6 Z_{14}}{C_A N^2}$$

$$\frac{\partial f_{15}}{\partial Z_1} = G_a \exp(\frac{-E_a}{RZ_7}) \frac{E_a}{RZ_7^2}(Z_9 - Z_{10})$$

$$\frac{\partial f_{15}}{\partial Z_2} = G_b \exp(\frac{-E_b}{RZ_7}) \frac{E_b}{RZ_7^2} Z_{10}$$

$$\frac{\partial f_{15}}{\partial Z_7} = G_a Z_1 (\frac{E_a}{RZ_7^2})^2 \exp(\frac{-E_a}{RZ_7})(Z_9 - Z_{10})$$

$$+ G_a Z_1 (\frac{-2E_a}{RZ_7^3}) \exp(\frac{-E_a}{RZ_7})(Z_9 - Z_{10})$$

$$+ G_b Z_2 (\frac{E_b}{RZ_7^2})^2 \exp(\frac{-E_b}{RZ_7}) Z_{10}$$

$$+ G_b Z_2 \exp(\frac{-E_b}{RZ_7})(\frac{-2E_b}{RZ_7^3}) Z_{10}$$

$$\frac{\partial f_{15}}{\partial Z_9} = G_a Z_1 (\frac{E_a}{RZ_7^2}) \exp(\frac{-E_a}{RZ_7})$$

$$\frac{\partial f_{15}}{\partial Z_{10}} = - G_a Z_1 (\frac{E_a}{RZ_7^2}) \exp(\frac{-E_a}{RZ_7}) + G_b Z_2 (\frac{E_b}{RZ_7^2}) \exp(\frac{-E_b}{RZ_7})$$

$$\frac{\partial f_{16}}{\partial Z_3} = (Z_{11} - Z_{12}) G_a \frac{E_a}{RZ_8^2} \exp(\frac{-E_a}{RZ_8})$$

$$\frac{\partial f_{16}}{\partial Z_4} = Z_{12} G_b (\frac{E_b}{RZ_8^2}) \exp(\frac{-E_b}{RZ_8})$$

$$\frac{\partial f_{16}}{\partial Z_8} = G_a Z_3 (\frac{E_a}{RZ_8^2})^2 \exp(\frac{-E_a}{RZ_8})(Z_{11} - Z_{12})$$

$$+ G_a Z_3 (\frac{-2E_a}{RZ_8^3}) \exp(\frac{-E_a}{RZ_8}) (Z_{11} - Z_{12})$$

$$+ G_b Z_4 \left(\frac{E_a}{RZ_8^2}\right)^2 \exp\left(\frac{-E_a}{RZ_8}\right) Z_{12}$$

$$+ G_b Z_4 \left(\frac{-2E_b}{RZ_8^3}\right) \exp\left(\frac{-E_b}{RZ_8}\right) Z_{12}$$

$$\frac{\partial f_{16}}{\partial Z_{11}} = G_a Z_3 \left(\frac{E_a}{RZ_8^2}\right) \exp\left(\frac{-E_a}{RZ_8}\right)$$

$$\frac{\partial f_{16}}{\partial Z_{11}} = - G_a Z_3 \left(\frac{E_a}{RZ_8^2}\right) \exp\left(\frac{-E_a}{RZ_8}\right) + G_b Z_4 \left(\frac{E_b}{RZ_8^2}\right) \exp\left(\frac{-E_b}{RZ_8}\right) \qquad (4\text{-}60)$$

For those elements which do not appear in above are all ual to zero.

Eq. (59) is a set of linear ordinary differential equations d with boundary conditions given by Eq. (33), (55), and (56). is problem can now be solved by the iterative procedure scribed earlier.

Since six fixed initial conditions are given, if the initial nditions for the particular and homogeneous solutions are osen to satisfy these given initial conditions, we can reduce e required homogeneous solutions from 16 sets to 10 sets. e general solution can be represented by

$$\overline{Z}(t) = \overline{Z}_p(t) + \sum_{m=1}^{10} a_m \overline{Z}_{H,m}(t) \qquad (4\text{-}61)$$

After obtaining the solutions of the 8 state variables and Lagrange multipliers, Eq. (24) and (50) can be solved for the ofit and the control variable A.

4-5 NUMERICAL ASPECTS

This problem was divided into five sub-problems for different values of the constants and initial conditions. The objective was to test the convergence and to investigate the other numerical aspects under different situations.

Problem A

The following values were assigned for the various parameters

$G_a = 0.535 \times 10^{11}$ per minute	$N = 100$
$G_b = 0.461 \times 10^{18}$ per minute	$C_c = 1$
$E_a = 18000$ cal./mole	$C_T = 0.001$ $\$/^oK$
$E_b = 30000$ cal./mole	$C_A = \$0.01$
$R = 2$ cal./mole ^oK	$C_1 = \$5.0$
$q = 60$ gal./min.	$C_2 = C_3 = \$0.0$
$V_1 = V_2 = 12$ gallons	$C_q = 1.0$
$I_m = 10$ gallons	$C_I = 1.0$ $/gal.
$T_{1m} = 340$ ^oK	$X_0(t_0) = 0.53$
$\Delta t = 0.02$	$y_0(t_0) = 0.43$

The boundary conditions were

$x_1(0) = 0.53$, $y_1(0) = 0.43$, $x_2(0) = 0.53$

$y_2(0) = 0.43$, $I(0) = 1.0$, $I(1) = 10.0$

$S(0) = 0.1$

It should be emphasized that problem A was the only problem which had final condition on the inventory.

Since most of the equations are nonlinear, hence initial approximations were required. The various sets of initial approximations used for this problem are listed in Table 1.

Problem B

The same parameters used in problem A were used here. Except that the final inventory was removed.

Different sets of initial approximations used are given in Table 2.

Problem C

Some of the parameters were changed. They are listed in below

$$C_T = 0.0005 \quad \$/^{o}K$$

$$C_A = \$\,0.0002$$

$$I_m = 20 \quad \text{gallons}$$

The boundary conditions are

$$x_1(0) = 0.53\,, \qquad y_1(0) = 0.43\,, \qquad x_2(0) = 0.53$$

$$y_1(0) = 0.43\,, \qquad I(0) = 8 \qquad S(0) = 0.1$$

A list of initial approximations is shown in Table 3.

Problem D

The problem is the same as problem C, except that

$C_A = 0.01$

and $S(0) = 1.0$ $I(0) = 15$

Three different initial approximations were used for this problem. They are listed in Table 4.

Problem E

The only difference between problem E and D is in the initial conditions. In this problem

$I(0) = 12$ $S(0) = 0.1$

All other values remain the same as in problem D. The values of the initial approximation used are given in Table 5.

The initial values used for the particular and homogeneous solutions are given in Table 6.

Problems A, B, and C were exactly the same as the first three problems in Chapter 5 of Shah's thesis [8]. The purpose of this is to compare the results under different situations, namely, to consider temperature as a function of t against as a constant parameter. The comparison of the results is given in a latter section.

4-6 COMPUTATIONAL ASPECTS

By using the initial values given in Table 6. and the initial approximations given in Tables 1 through 5, the system can be solved numerically. A set of particular solutions and 10 sets of homogeneous solutions were obtained by the Runge-Kutta integration method.

Ten integration constants were obtained after the calculation of particular and homogeneous solutions, and the substitution of the boundary conditions. In order to solve these ten integration constants on the computer, the subroutine DGELG, which is a double-precisioned subroutine programmed for solving simultaneous linear algebraic equations, was used.

Using these integration constants, the general solutions for all 16 variables can be obtained by Eq. (61). By using Eq. (50), values of advertisement at all grid points were obtained.

For simplicity the following approximation was used to calculate the total profit

$$J = \sum_{t_0}^{t_f} [C_1 C_q S + C_2 q x_2 + C_3 a(1 - X_2 - y_2) - C_I(I_m - I)^2$$

$$- C_A A^2 S^2]\, t - C_T[(T_{1m} - T_1(0))^2 + (T_1(0) - T_2(0))^2]$$

Since the temperature greatly influences the performance equations, at the first few iterations, a too high or too low temperature may cause exponential overflow on the computer. Hence a limit was set for the temperature to insure convergence

$$300^\circ \leq T_1 , T_2 \leq 370^\circ$$

This limit was used for all five problems

At first, problem A was solved on the computer using single-precision scheme. But the solutions converged very slowly after the convergence had already taken place. For the quasilinearization technique, owing to the use of the Newton-Raphson type of linearization formula, the convergence should be quadratic if the convergence exists. After changing to double-precision scheme on the computer, this slow convergence did not exist any more. One explanation for this situation is due to the highly nonlinear terms in the performance equations. These terms may cause the problem to be unstable, and thus make the solution fluctuate.

The computer program used for solving these five sub-problems is given in Appendix 1. It consists of a main program with three subroutines. The subroutine RUNGK which is essentially the Runge-Kutta method, was first written in a very general form. It can handle a set of differential equations of any number. But later on, it was found that this integration subroutine required too much execution time. After modifying this RUNGK routine, the total computer time required decreased by half.

All the five problems were solved on the IBM-360-50 using double precision accuracy. The computer time required for each problem using FORTRAN 4, G level complier is approximately 20 minutes for 11 iterations.

4-7 RESULTS

The results of all the sub-problems from A to E are given separately in the following pages.

Problem A

All the three initial approximations listed in Table 1 converged to the optimal solution.

The convergence rates of the six state variables and one control variable for problem 1A are shown in Fig. 1 through 7. The optimal profiles of Lagrange multipliers are shown in Fig. 8 to 10. Table 7 gives the convergence rate of T_1, T_2, $S(t_f)$ and profit. In Table 8, convergence rate of A(t) is given. The profit of this problem was $80.062.

Generally speaking, there is no convergence difficulty encountered in this problem. The initial approximations used for problem 1A, 2A, and 3A were quite arbitrary and far different from one to another.

A comparison of the optimal profiles and the convergence rate of A(0) with Shah's [8] results are given in Tables 9 and 10.

Although the profit we got in the present method is a little higher than Shah's result, it was simply caused by the accuracy used on the computer. Shah used 100 grid points and single precision. In our case, 50 grid points and double precision were used. To clear this doubt, the results were recalculated using 100 grid points and single precision. The profit we got was 79.67, compared with Shah's 79.75 or about 0.07 less. In Table 10, the convergence rate is a little faster in our case which is the result of double precision accuracy.

Problem B

All the five initial approximations given in Table 2 converged to the optimal solution. No convergence difficulty existed. It seems that any reasonable guess will make this problem converge.

The optimal profiles of the state variables and the control variable are shown in Figs. 11 and 12. In Table 11, the convergence rate of T_1, T_2, $I(t_f)$, $S(t_f)$, and profit J are given. Table 12 shows the convergence rate of A(t).

The total profit of this problem is $96.09 which is also more than what Shah had. In his results, the profit was $95.79. This is also caused by the accuracy used on the computer.

Since Shah did not give any convergence figure of the variables for this problem, no comparison can be given except the profit.

Problem C

Among the four initial approximations, only 1C and 3C converged to the optimal solution.

Figs. 13 to 18 show the convergence rates of the six state variables and one control variable. In Table 13, the convergence rate of T_1, T_2, $I(t_f)$, $S(t_f)$, and J are given. Table 14 gives the convergence rate of A(t).

In this problem, C_A changed from \$0.01 to \$0.0002 and C_T changed from \$0.001 to \$0.0005, both of them decreased a lot. These changes actually put more weight on the cost of the inventory. Since $I_{1m} = 20$ and $I(0) = 8$, the process tends to increase the inventory by decreasing the sales. This is the reason why there are negative sales shown in Fig. 20. These negative sales, of course, are caused by having negative advertisement which is unreasonable in real situations.

Although the optimal solution for this problem is unreasonable, but it did converge rapidly in 7 iterations. This is merely another proof of the powerfulness of quasilinearization. In Shah's thesis, this problem did not converge using two different initial approximations. He also tried to change the initial values of sales. For all of the cases he tried, the Newton-Raphson convergence difficulty was encountered in the first iteration.

Problem 2C did not converge because too low temperatures were obtained in first iteration. After using the limits to set them at 300°, the temperatures still did not go up.

In problem 3C, the initial inventory, I(0) was increased from 8 to 15. It was hoped that this change could avoid the negative sales. Unfortunately, there were still negative sales and advertisement existing.

Problem D

Three initial approximations were used for this problem. Only the first one did not converge. 2D and 3D converged in 9 iterations.

The convergence rates of the state and control variables are shown in Figs. 19 to 24. Tables 15 and 16 show the convergence rates of T_1, T_2, $I(t_f)$, $S(t_f)$, J, and A(t).

The convergence rate of this problem is slow as far as the number of iterations is concerned. It was probably caused by the small value of C_T which made the temperature fluctuate.

Problem 1D encountered the same difficulty which happened in problem 2C.

Problem E

The three initial approximations used for this problem are given in Table 5. All of them converged to the optimal solution.

The optimal profiles of this problem are shown in Figs. 25 and 26. Table 17 shows the convergence rate of T_1, T_2, $I(t_f)$, $S(t_f)$, and J. The convergence rate of A(t) is given in Table 8.

The convergence rate of this problem is about the same as in problem D. An average of 10 iterations is required for the convergence of the three problems.

One interesting fact which can be found in Table 17 is the convergence rate of T_2. At the first iteration, T_2 had the value of -800.97. In spite of the highly nonlinear nature of T_2 and a value far off from the true solution, it finally converged to the optimal solution.

4-8 DISCUSSION

The results of all the problems indicate that considering temperature as a constant parameter is superior to considering it as a function of t. There are mainly two advantages for the present method. First, to maintain the temperature at a fixed constant value is much easier than to control it according to a fixed function of t. Besides this, the loss of profit using the present approach is negligible. Fig. 27 shows a comparison of optimal profiles of the temperatures under the two different approaches. Shah had the optimal temperature ranging approximately from 365° at (t_0) to 340° at (t_f). For the present method, both T_1 and T_2 were around 360°. Second, no convergence difficulty existed in general. Since temperature is a constant parameter and can be considered as additional state variable, the Newton-Raphson convergence difficulty which Shah had in finding T_1 and T_2 did not occur in our case.

Comparing the optimal solutions of all the problems, it was observed that the values of parameters C_A, C_I, and C_T did influence the solution. Generally speaking, when $C_A = 0.01$, reasonable curves were obtained for the advertisement. A small value of C_A caused advertisement to be either negative or discontinuous. As for C_I, a relatively high value of this parameter made the process tend to maintain the inventory as close to I_m as possible. This tendency caused the solution to have negative sales as well as negative advertisement. The influences of C_T can be observed in problems D and E. Both of these two problems have slow convergence rate. It was mainly because of the unstability of the model caused by small value of C_T.

Another interesting fact is the relationship among I(0), S(0), and A(t). The appearance of large amount advertisement at the begining is caused by small S(0) and large I(0). While negative advertisement is usually caused by large S(0) and small I(0).

In general, convergence was obtained in 6 to 7 iterations for the first three problems. 8 to 9 iterations for the last two problems. The accuracy required for convergence was three digits after the decimal point for most of the problems. The convergence rate was almost independent of the choice of initial approximation for the values used in this work.

Table 1. Initial approximations for problem A

Set No.	$X_1(t)$	$y_1(t)$	$x_2(t)$	$y_2(t)$	$I(t)$	$S(t)$	$T_1(t)$	$T_2(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$	$\lambda_7(t)$	$\lambda_8(t)$
1A	0.53	0.43	0.53	0.43	1.0	1.0	340	340	-5	-20	-5	-40	-8	0.0	1.0	1.0
2A	0.53	0.43	0.53	0.43	0.0	30	330	330	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
3A	0.53	0.43	0.53	0.43	0.0	50	345	345	-2	-2	-2	-2	-2	-2	-2	-2

Table 2. Initial approximations for problem B

Set No.	$x_1(t)$	$y_1(t)$	$x_2(t)$	$y_2(t)$	$I(t)$	$S(t)$	$T_1(t)$	$T_2(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$	$\lambda_7(t)$	$\lambda_8(t)$
1B	0.53	0.43	0.53	0.43	0	0	340	340	-5	-5	-5	-5	-5	0.0	1.0	1.0
2B	0.53	0.43	0.53	0.43	0	0	340	340	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
3B	0.53	0.43	0.53	0.43	1	1	330	330	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4B	0.53	0.43	0.53	0.43	2	2	345	345	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1	-0.1
5B	0.53	0.43	0.53	0.43	1	1	340	340	-5	-20	-5	-40	-8	0.0	1.0	1.0

Table 3. Initial approximations for problem C

Set No.	$x_1(t)$	$y_1(t)$	$x_2(t)$	$y_2(t)$	$I(t)$	$S(t)$	$T_1(t)$	$T_2(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$	$\lambda_7(t)$	$\lambda_8(t)$
1C	0.53	0.43	0.53	0.43	3	1	340	340	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5
2C	0.53	0.43	0.53	0.43	1	3	345	345	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
3C	0.53	0.43	0.53	0.43	1	3	345	345	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Table 4. Initial approximations for problem D

Set No.	$x_1(t)$	$y_1(t)$	$x_2(t)$	$y_2(t)$	$I(t)$	$S(t)$	$T_1(t)$	$T_2(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$	$\lambda_7(t)$	$\lambda_8(t)$
1D	0.53	0.43	0.53	0.43	20	15	335	335	-2	-10	-2	-10	-2	-1	-1	-1
2D	0.53	0.43	0.53	0.43	1	3	340	340	1	1	1	1	1	1	1	1
3D	0.53	0.43	0.53	0.43	20	10	345	345	-1	-4	-1	-9	-3	-1	-0.1	-0.1

Table 5. Initial approximations for problem E

Set No.	$x_1(t)$	$y_1(t)$	$x_2(t)$	$y_2(t)$	$I(t)$	$S(t)$	$T_1(t)$	$T_2(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$	$\lambda_7(t)$	$\lambda_8(t)$
1E	0.53	0.43	0.53	0.43	20	15	345	345	0	-2	0	-5	-1	0.0	0.5	0.5
2E	0.53	0.43	0.53	0.43	18	10	350	350	-5	-10	-5	-15	-5	-1	0.0	0.0
3E	0.53	0.43	0.53	0.43	10	20	355	355	-3	-15	-2	-20	-2	-1.5	-0.005	0.01

Table 6. Initail values used for particular and homogeneous solutions

	P.I. for A,B	P.I. for C	P.I. for D	P.I. for E	Homogeneous solutions									
					1	2	3	4	5	6	7	8	9	10
$x_1(0)$	0.53	0.53	0.53	0.53	0	0	0	0	0	0	0	0	0	0
$y_1(0)$	0.43	0.43	0.43	0.43	0	0	0	0	0	0	0	0	0	0
$x_2(0)$	0.53	0.53	0.53	0.53	0	0	0	0	0	0	0	0	0	0
$y_2(0)$	0.43	0.43	0.43	0.43	0	0	0	0	0	0	0	0	0	0
$I(0)$	1.0	8.0	15	12	0	0	0	0	0	0	0	0	0	0
$S(0)$	0.1	0.1	1.0	1.0	0	0	0	0	0	0	0	0	0	0
$T_1(0)$	0	0	0	0	1	0	0	0	0	0	0	0	0	0
$T_2(0)$	0	0	0	0	0	1	0	0	0	0	0	0	0	0
$\lambda_1(0)$	0	0	0	0	0	0	1	0	0	0	0	0	0	0
$\lambda_2(0)$	0	0	0	0	0	0	0	1	0	0	0	0	0	0
$\lambda_3(0)$	0	0	0	0	0	0	0	0	1	0	0	0	0	0
$\lambda_4(0)$	0	0	0	0	0	0	0	0	0	1	0	0	0	0
$\lambda_5(0)$	0	0	0	0	0	0	0	0	0	0	1	0	0	0
$\lambda_6(0)$	0	0	0	0	0	0	0	0	0	0	0	1	0	0
$\lambda_7(0)$	0	0	0	0	0	0	0	0	0	0	0	0	1	0
$\lambda_8(0)$	0	0	0	0	0	0	0	0	0	0	0	0	0	1

Table 7. Convergence Rates of T_1, T_2, $S(t_f)$, and J, problem 1A

ITER.	0	1	2	3	4	5	6	7
T_1	340.0	396.03	366.76	361.99	359.74	359.23	359.21	359.21
T_2	340.0	297.52	467.61	363.58	360.99	360.34	360.30	360.30
$S(t_f)$	1.0	34.61	33.38	35.25	34.87	34.76	34.76	34.76
J	-	58.518	65.395	81.430	80.364	80.074	80.062	80.062

Table 8. Convergence Rates of A(t) in problem 1A

TIME ITER.	1	2	3	4	5	6	7
0.0	214.10	320.74	382.28	371.90	368.92	368.78	368.78
0.2	4.71	4.75	4.63	4.67	4.67	4.67	4.67
0.4	1.49	1.74	1.70	1.71	1.72	1.72	1.72
0.6	0.48	0.69	0.68	0.68	0.68	0.68	0.68
0.8	0.11	0.22	0.22	0.22	0.22	0.22	0.22
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 9. A comparison of the optimal profiles of problem A with Shah's results

	J	$T_1(0)$	$T_1(t_f)$	$T_2(0)$	$T_2(t_f)$	A(0)	$A(t_f)$
Shah's	79.75	362.4	340.0	365.7	340.0	370.4	0.00
Prob. A	80.06	359.21	359.21	360.30	360.30	368.78	0.00

Table 10. A Comparison of the Convergence Rate of A(0) in problem A with Shah's result

ITER.	Shah's	1A	2A	3A
1	260.40	214.10	844.48	611.86
2	358.80	320.74	428.15	376.78
3	366.40	382.28	372.18	384.36
4	370.60	371.90	369.01	370.69
5	369.90	368.92	368.78	368.82
6	370.50	368.78	368.78	368.78
7	370.30	368.78	368.78	368.78
8	370.40	368.78	368.78	368.78

Table 11. Convergence Rates of T_1, T_2, $I(t_f)$, $S(t_f)$, and J, in problem B

ITER.	0	1	2	3	4	5	6	7
T_1	345.0	413.90	366.14	361.64	359.78	359.45	359.44	359.44
T_2	345.0	456.82	367.73	363.15	361.29	360.95	360.93	360.93
$I(t_f)$	2.0	- 3.02	2.35	2.55	2.49	2.48	2.48	2.48
$S(t_f)$	2.0	85.68	49.91	48.79	48.47	48.43	48.43	48.43
J	-	147.77	96.43	97.38	96.24	96.10	96.09	96.09

Table 12. Convergence Rate of A(t) in problem B

ITER / Time	1	2	3	4	5	6	7
0.0	463.81	483.21	495.83	481.38	479.41	479.36	479.36
0.2	4.28	4.98	4.97	5.00	5.00	5.00	5.00
0.4	1.43	2.13	2.12	2.13	2.13	2.13	2.13
0.6	0.54	1.10	1.09	1.09	1.10	1.10	1.10
0.8	0.16	0.50	0.50	0.50	0.50	0.50	0.50
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 13. Convergence Rates of T_1, T_2, $I(t_f)$, $S(t_f)$, and J, in problem 1C

ITER.	0	1	2	3	4	5	6	7
T_1	330.0	519.12	363.39	360.83	360.05	360.00	360.00	360.00
T_2	330.0	628.79	364.70	361.84	360.52	360.34	360.34	360.34
$I(t_f)$	3	13.77	5.24	3.80	3.77	3.77	3.77	3.77
$S(t_f)$	1	28.87	67.35	81.36	82.64	82.67	82.67	82.67
J	-	47.924	110.533	113.843	113.495	113.459	113.458	113.458

Table 14. Convergence Rate of A(t) in problem 1C

Time \ ITER.	1	2	3	4	5	6	7	8
0.0	76.84	-7211.40	-5281.72	-5203.55	-5582.04	-5584.07	-5583.87	-5583.89
0.2	23.12	-11.51	-17.59	-19.12	-19.18	-19.18	-19.18	-19.18
0.4	17.53	5.97	6.33	6.28	6.28	6.29	6.29	6.29
0.6	14.66	5.18	4.41	4.50	4.49	4.49	4.49	4.49
0.8	12.21	4.89	3.46	3.41	3.41	3.41	3.41	3.41
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 15. Convergence Rates of T_1, T_2, $I(t_f)$, $S(t_f)$, and J, in problem D

ITER.	0	1	2	3	4	5	6	7	8	9	10
T_1	340.0	170.78	165.55	348.03	367.03	398.45	363.44	360.64	359.90	359.85	359.95
T_2	340.0	454.00	320.06	304.22	429.9	362.31	360.33	360.53	360.56	360.56	360.56
$I(t_f)$	1	3.09	4.22	10.94	10.45	11.30	11.80	11.83	11.82	11.82	11.82
$S(t_f)$	3	-10.66	72.67	50.31	47.81	51.73	52.85	52.82	52.79	52.79	52.79
J		-412.86	119.98	116.50	91.84	119.54	125.36	125.30	125.21	125.21	125.21

Table 16. Convergence Rate of A(t) in problem D

Time \ ITER.	1	2	3	4	5	6	7	8	9
0.0	-156.16	29.91	74.50	63.34	80.34	85.92	85.87	85.73	85.72
0.2	6.16	0.04	3.73	4.03	3.97	4.01	4.02	4.02	4.02
0.4	1.56	-0.01	1.54	1.74	1.65	1.66	1.67	1.67	1.67
0.6	-0.67	0.15	0.86	0.95	0.86	0.86	0.86	0.86	0.86
0.8	-2.03	0.15	0.44	0.47	0.42	0.41	0.41	0.41	0.41
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 17. Convergence Rates of T_1, T_2, $I(t_f)$, $S(t_f)$, and J, problem 1E

ITER	0	1	2	3	4	5	6	7	8	9	10
T_1	345.0	-75.92	270.17	325.24	284.62	376.65	363.33	360.76	360.14	360.09	360.09
T_2	345.0	-800.97	304.70	274.63	362.65	361.63	360.78	360.82	360.85	360.85	360.85
$I(t_f)$	2.0	7.10	-0.43	10.44	11.71	12.08	12.31	12.32	12.32	12.32	12.32
$S(t_f)$	15	-82.55	108.91	48.81	46.65	48.74	49.63	49.59	49.56	49.56	49.56
J	-	-940.12	121.97	97.19	89.09	101.01	104.76	104.60	104.53	104.52	104.52

Table 18. Convergence Rate of A(t), problem 1E

Time \ ITER	1	2	3	4	5	6	7	8	9	10
0.0	-3108.18	-196.72	464.70	459.74	547.32	589.16	587.03	585.93	585.86	585.86
0.2	6.12	-14.45	3.43	4.94	4.77	4.73	4.74	4.74	4.74	4.74
0.4	1.51	-1.45	1.27	2.13	2.02	1.99	2.00	2.00	2.00	2.00
0.6	-0.21	-0.13	0.84	1.12	1.05	1.03	1.03	1.03	1.03	1.03
0.8	-0.63	0.06	0.49	0.53	0.49	0.48	0.48	0.48	0.48	0.48
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

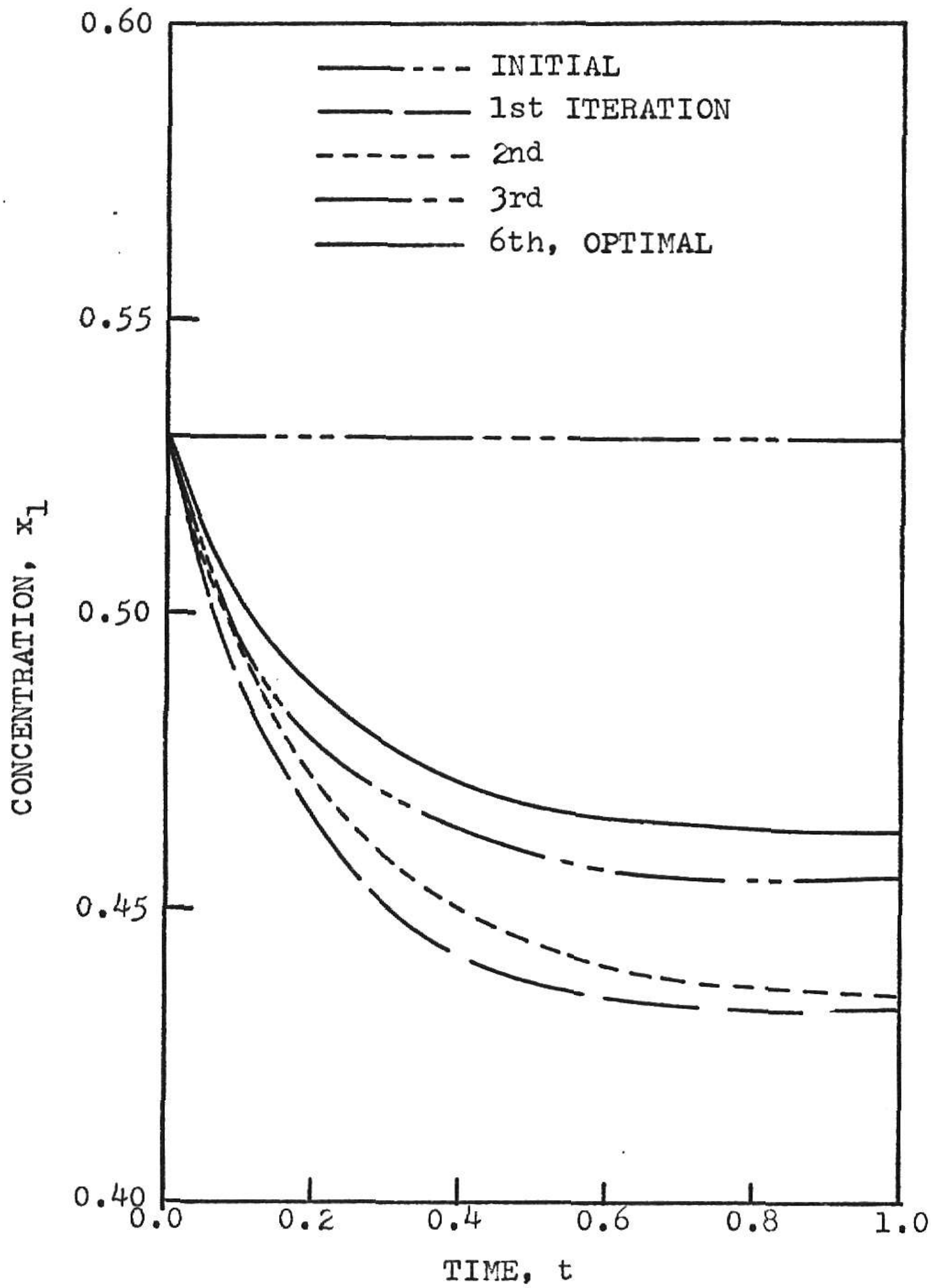

Fig. 1. Convergence Rate of Concentration x_1, Problem 1A

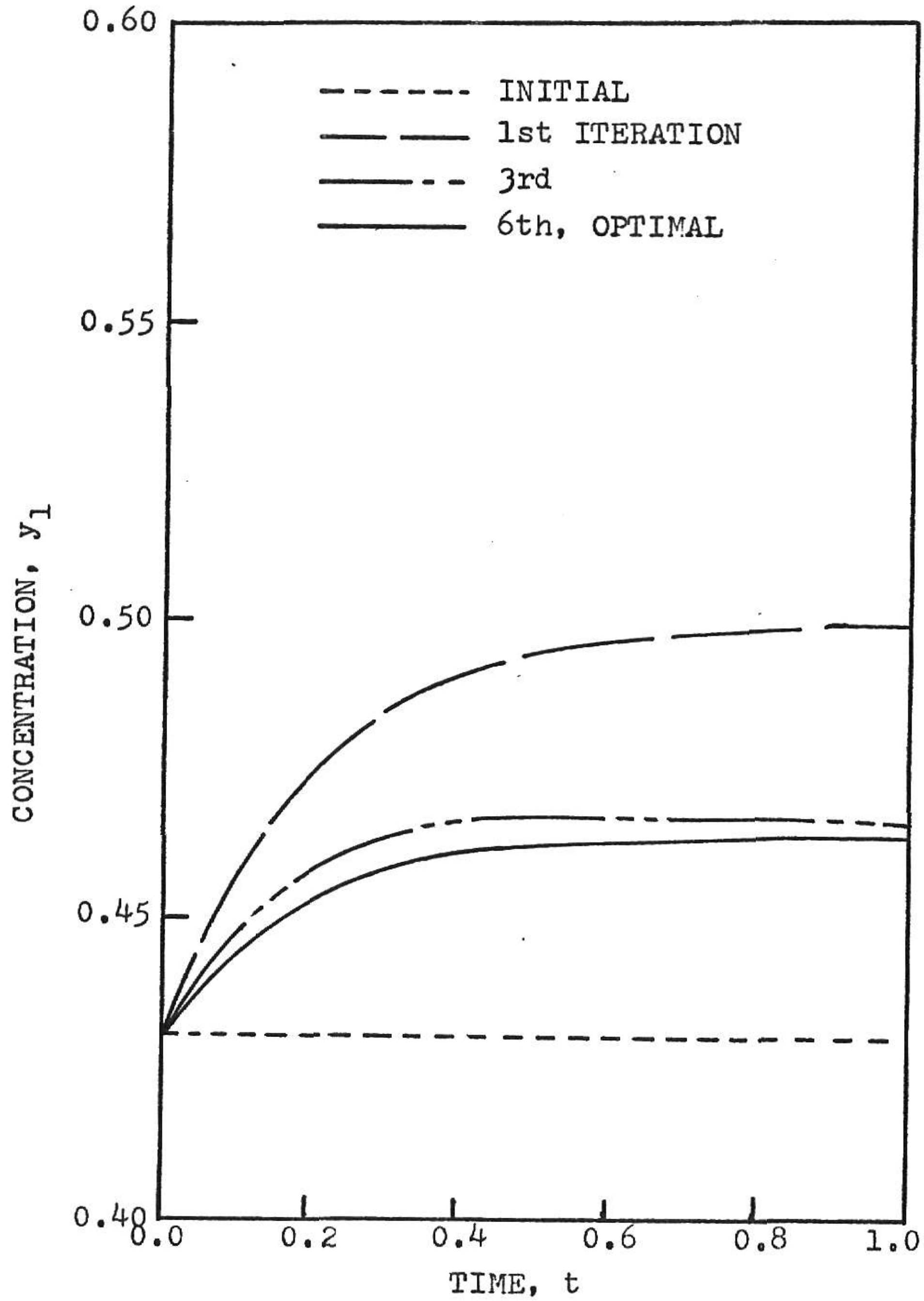

Fig. 2. Convergence Rate of Concentration y_1, Problem 1A

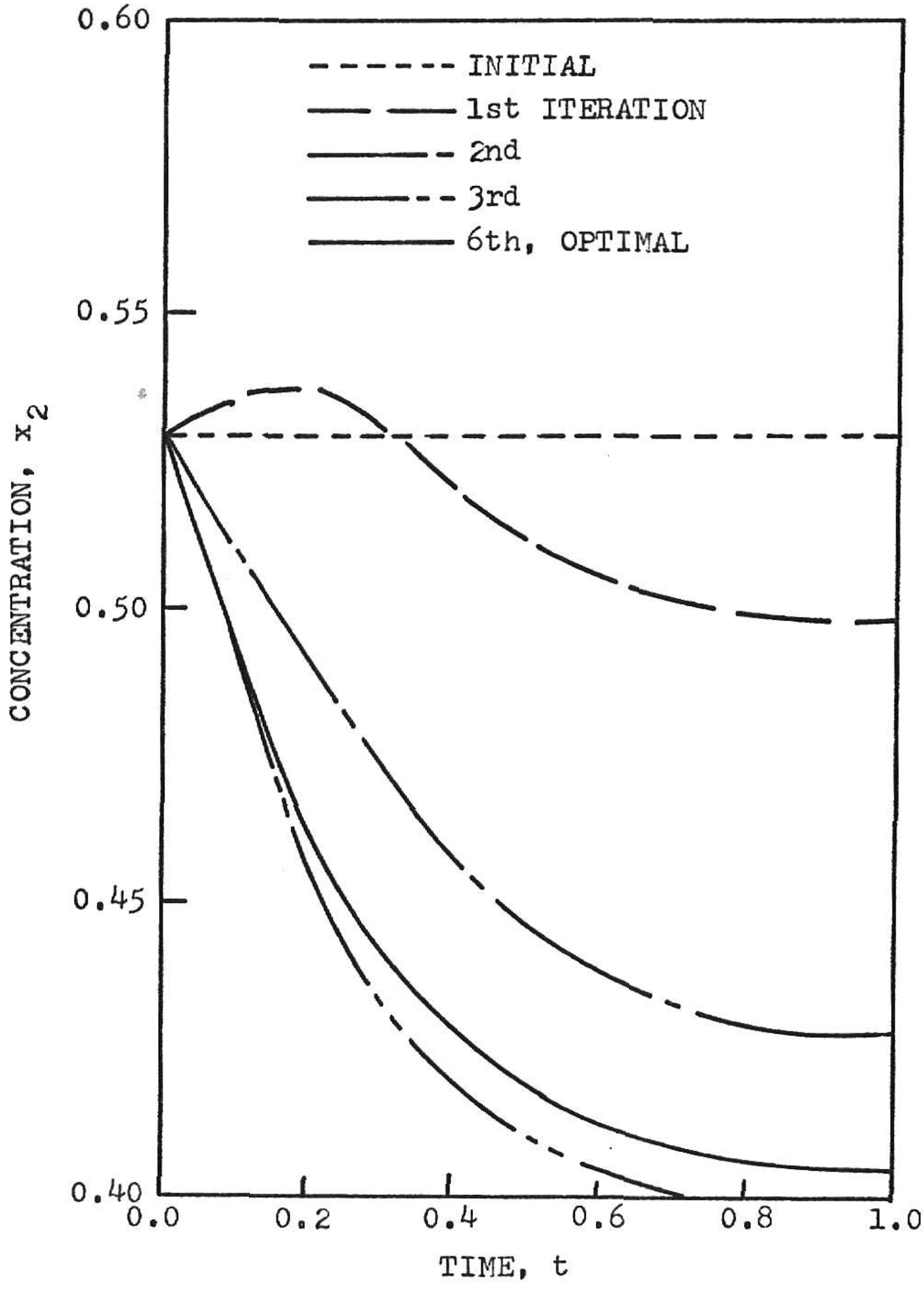

Fig. 3. Convergence Rate of Concentration x_2, Problem 1A

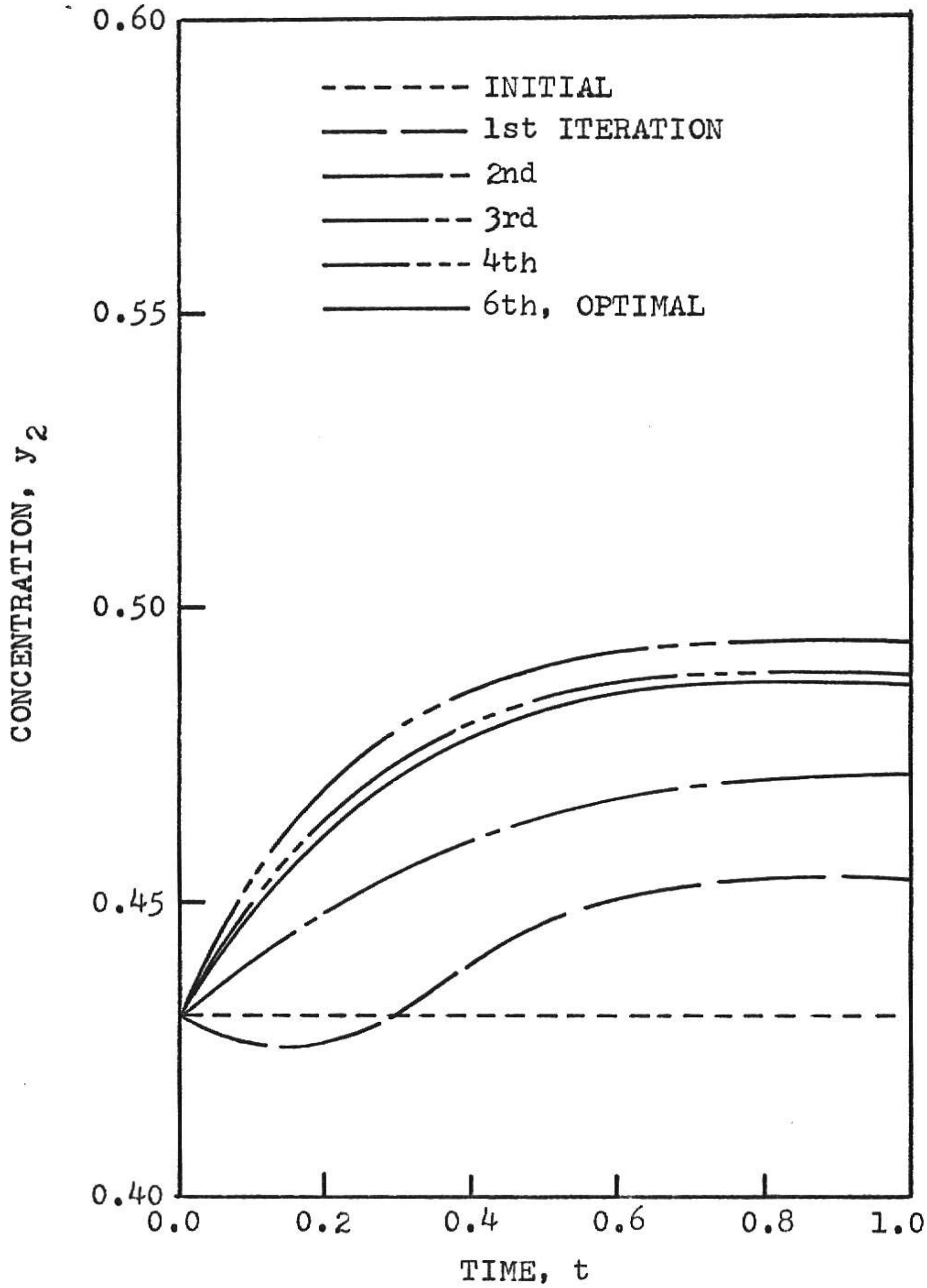

Fig. 4. Convergence Rate of Concentration y_2, Problem 1A

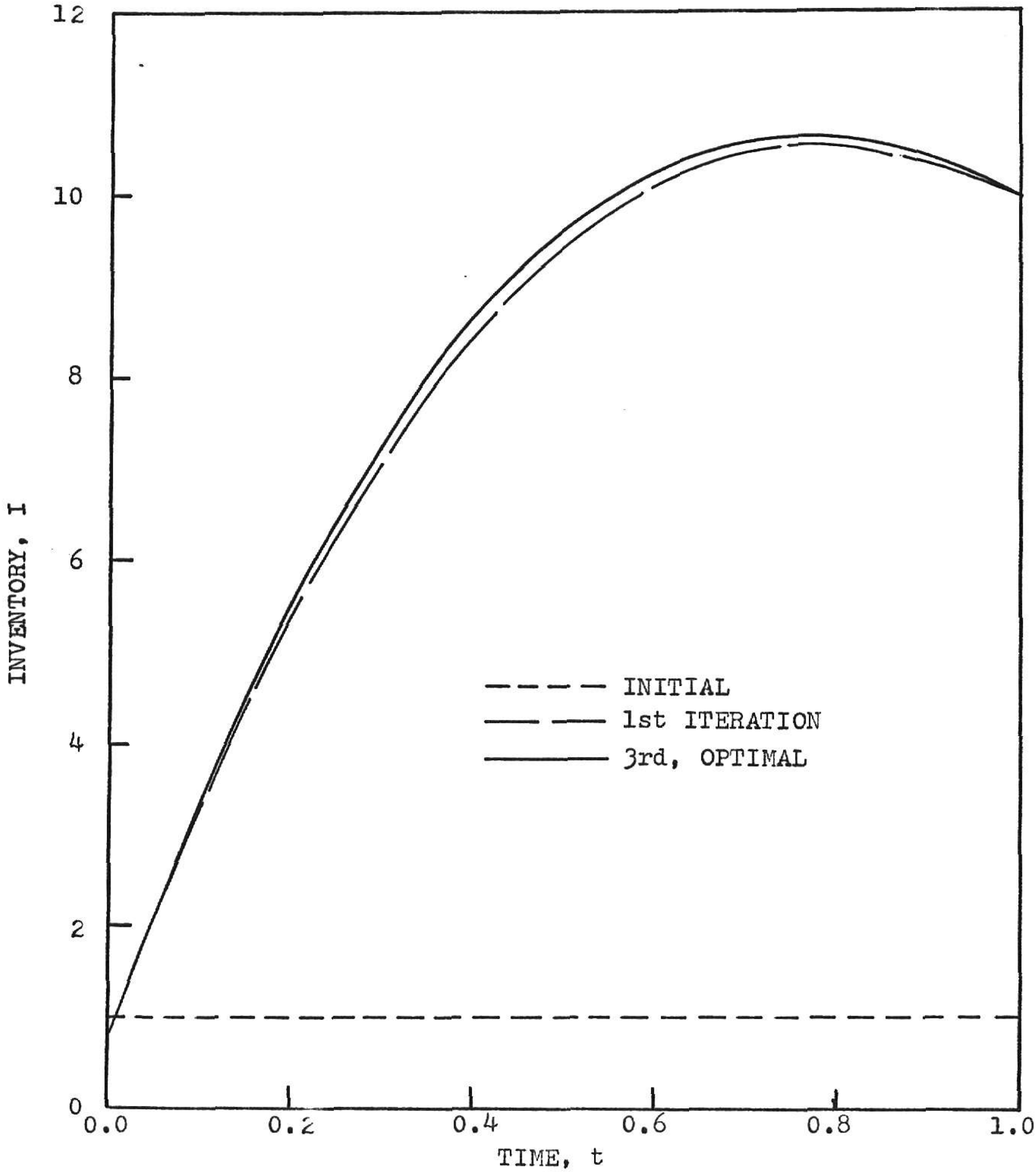

Fig. 5. Convergence Rate of Inventory I, Problem 1A

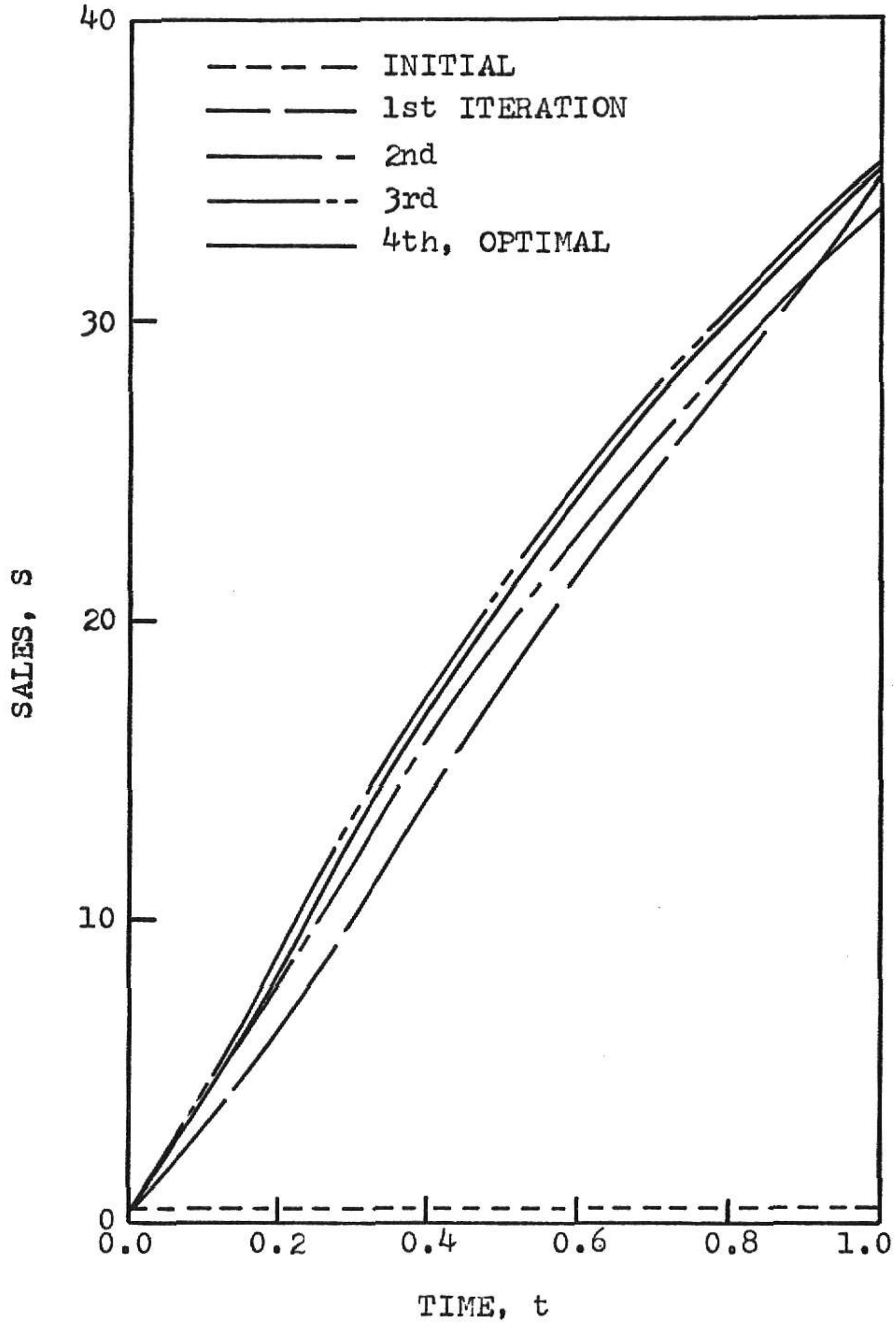

Fig. 6. Convergence Rate of Sales S, Problem 1A

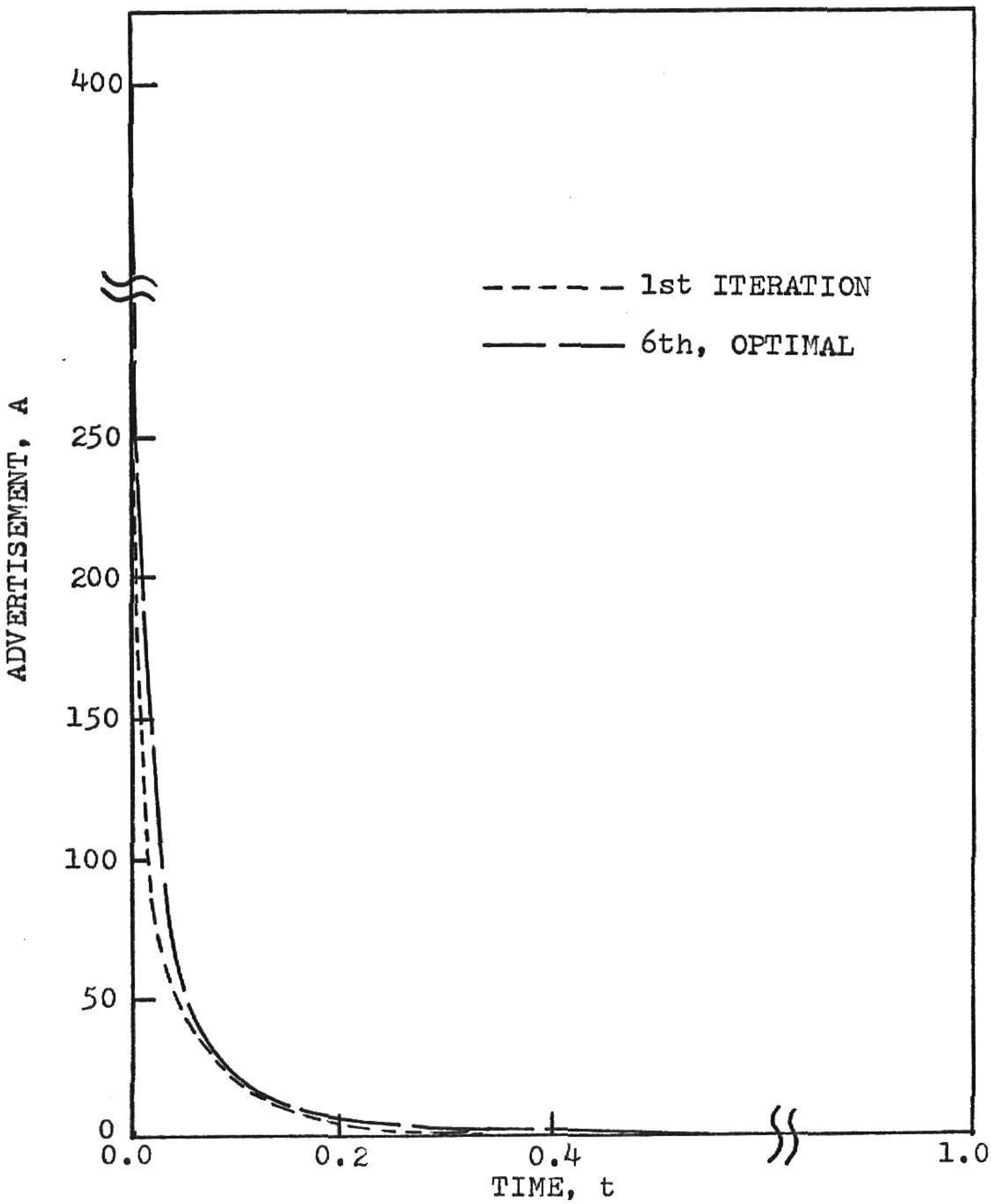

Fig. 7. Convergence Rate of Advertisement A, Problem 1A

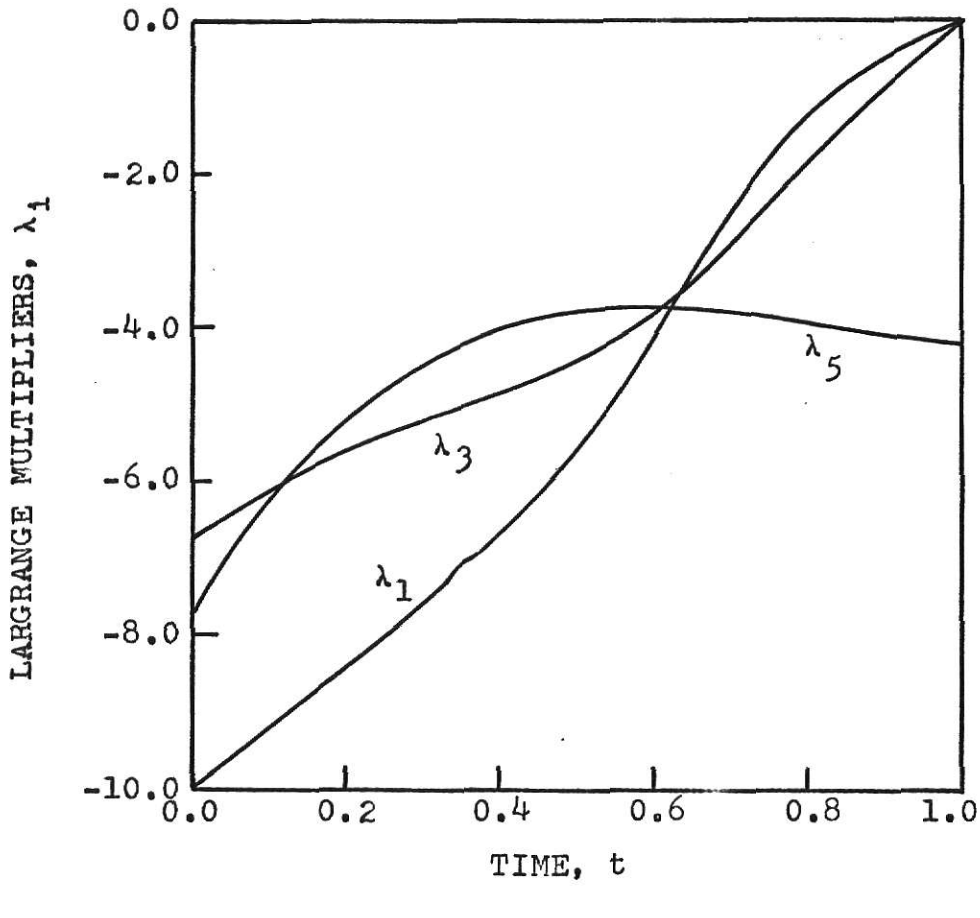

Fig. 8. Optimal Profiles of λ_1, λ_3, and λ_5, Problem 1A

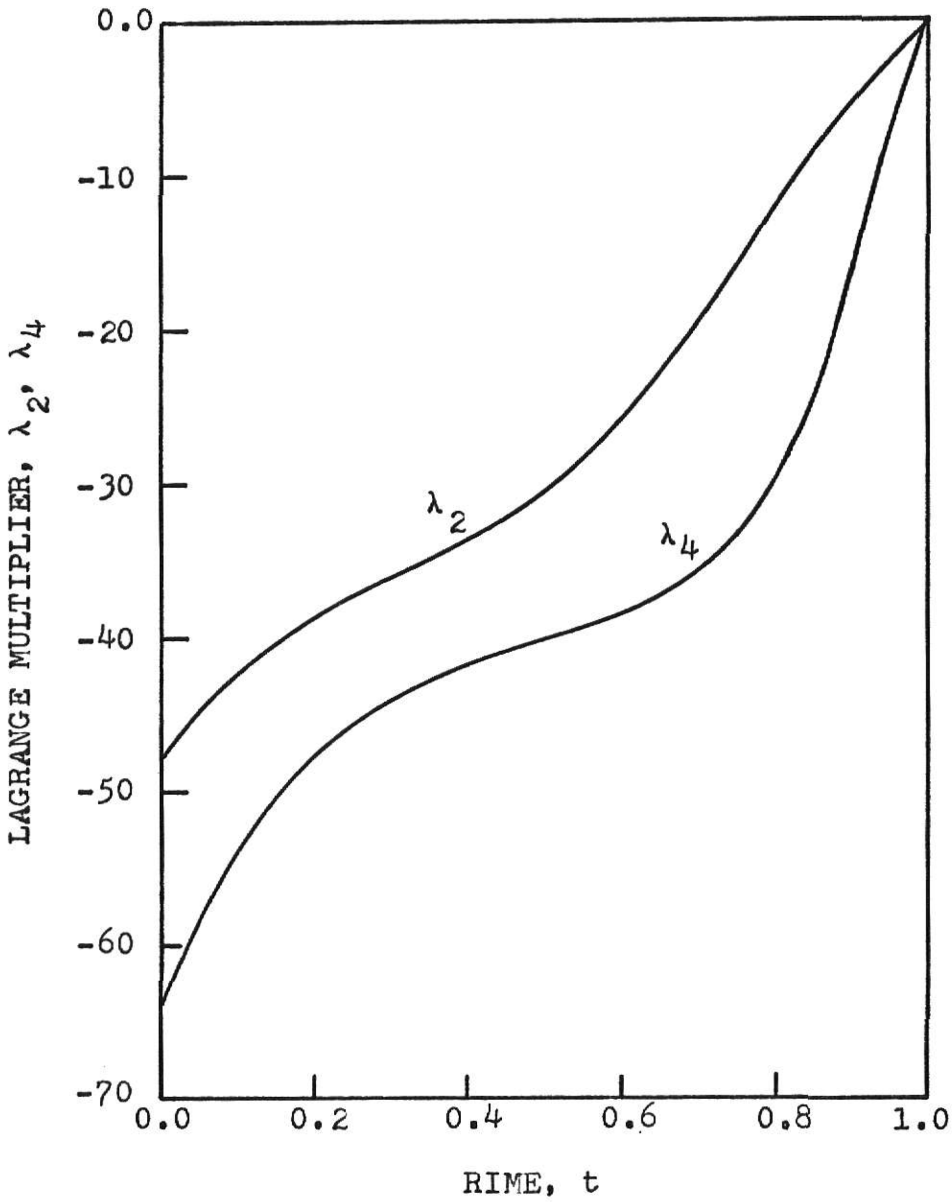

Fig. 9. Optimal Profiles of λ_2 and λ_4, Problem 1A

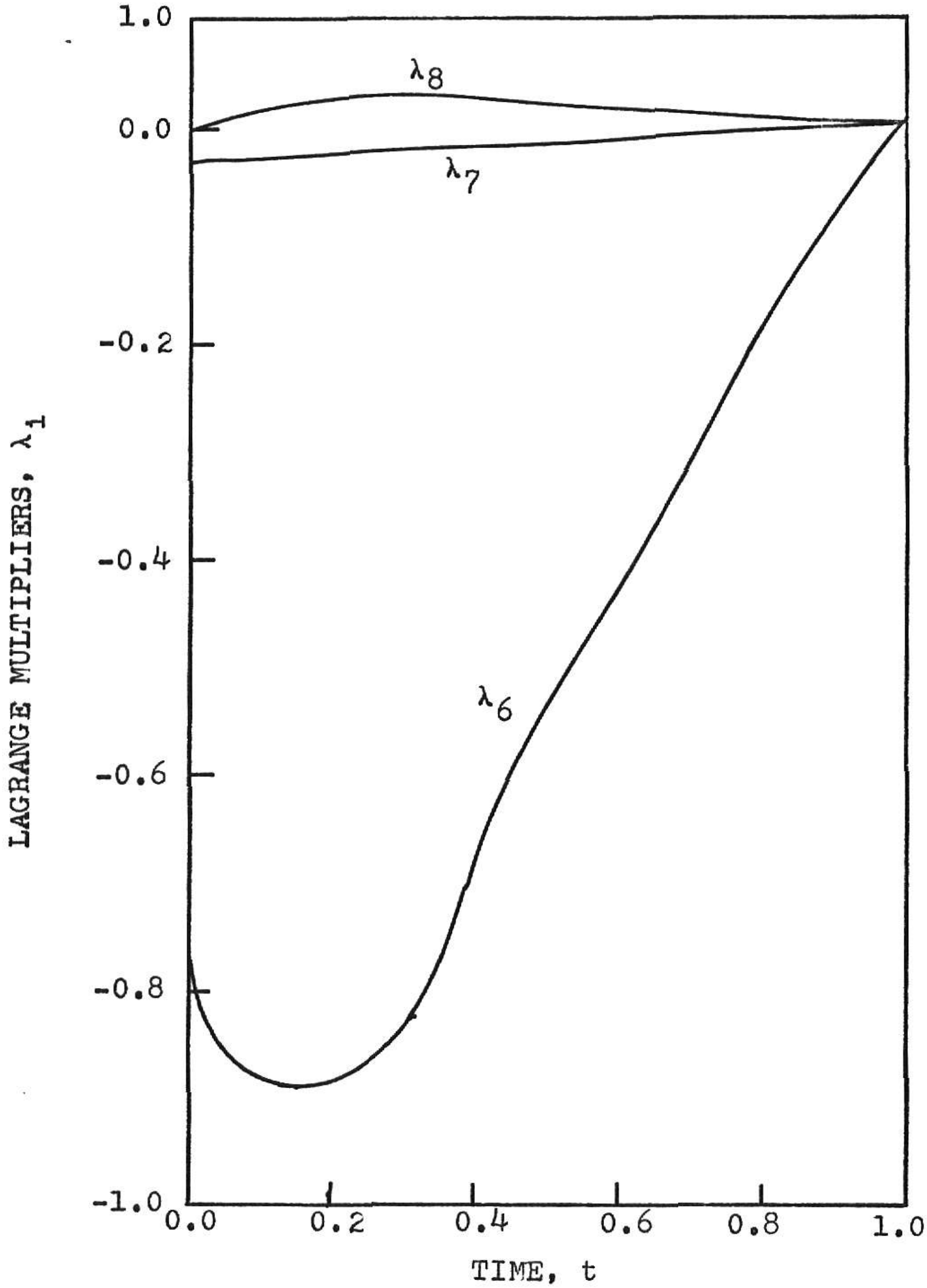

Fig. 10. Optimal Profiles of λ_6, λ_7, and λ_8, Problem 1A

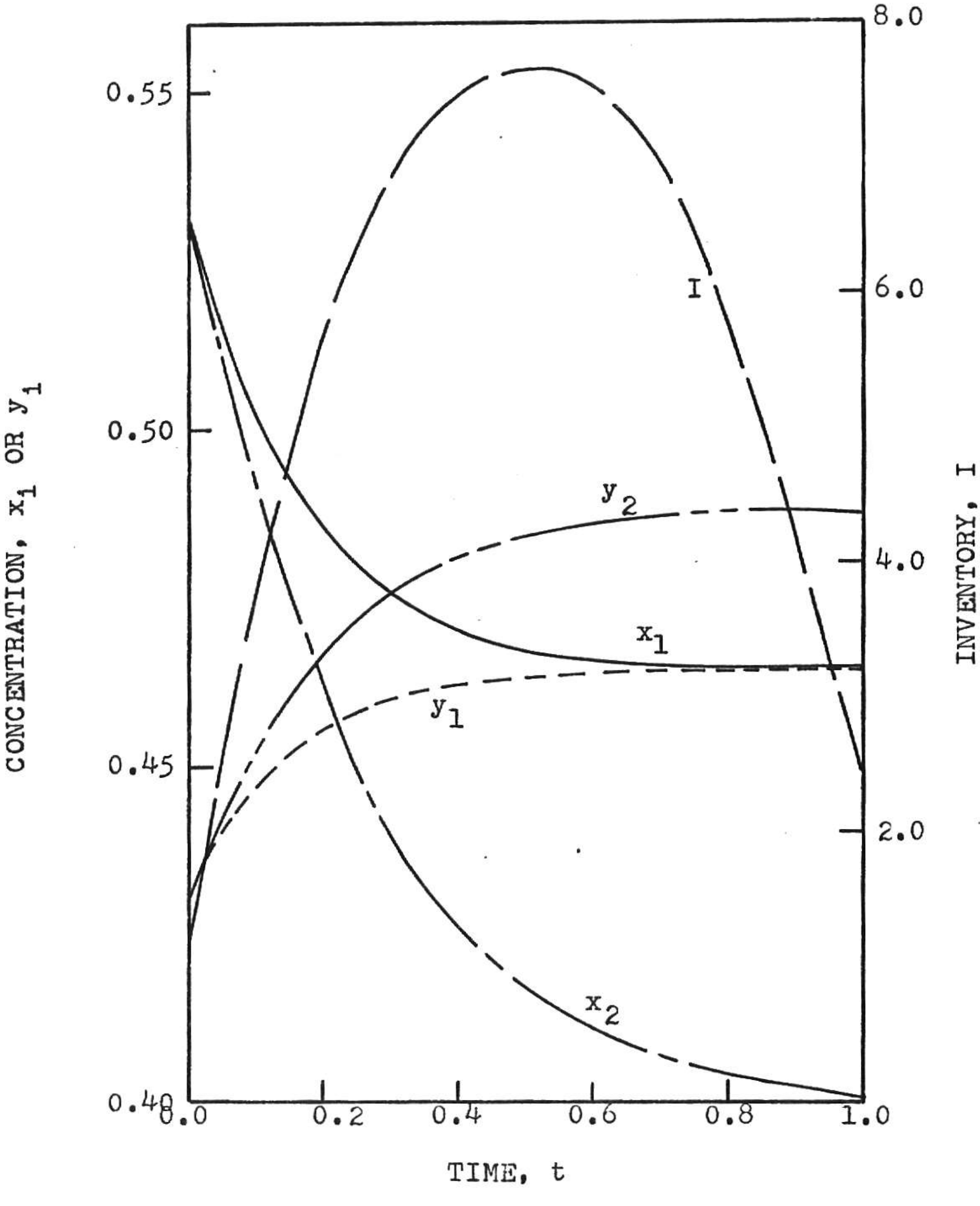

Fig. 11. Optimal Solutions of x_1, y_1, x_2, y_2, and I, Problem B

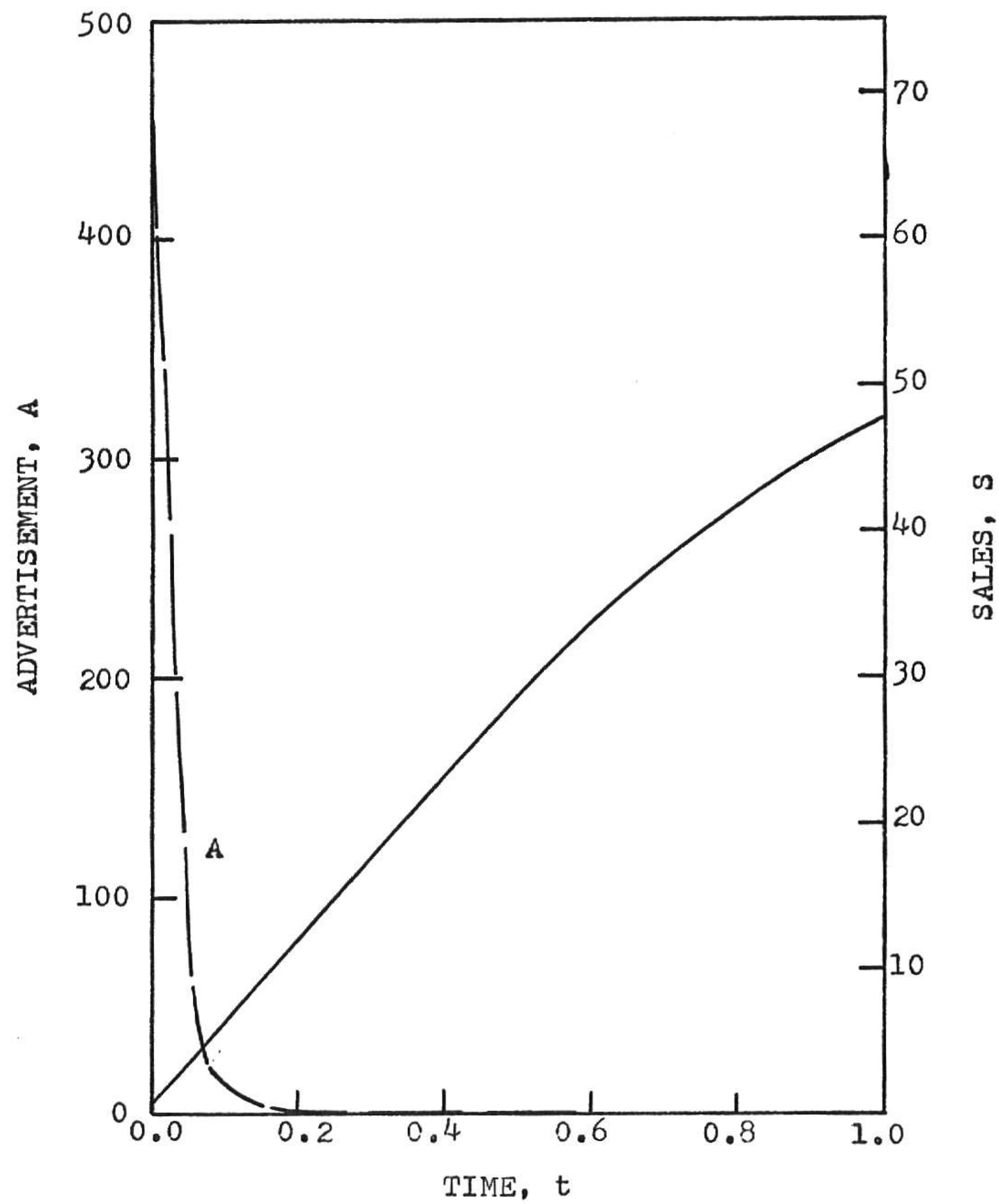

Fig. 12. Optimal Profiles of A and S, Problem B

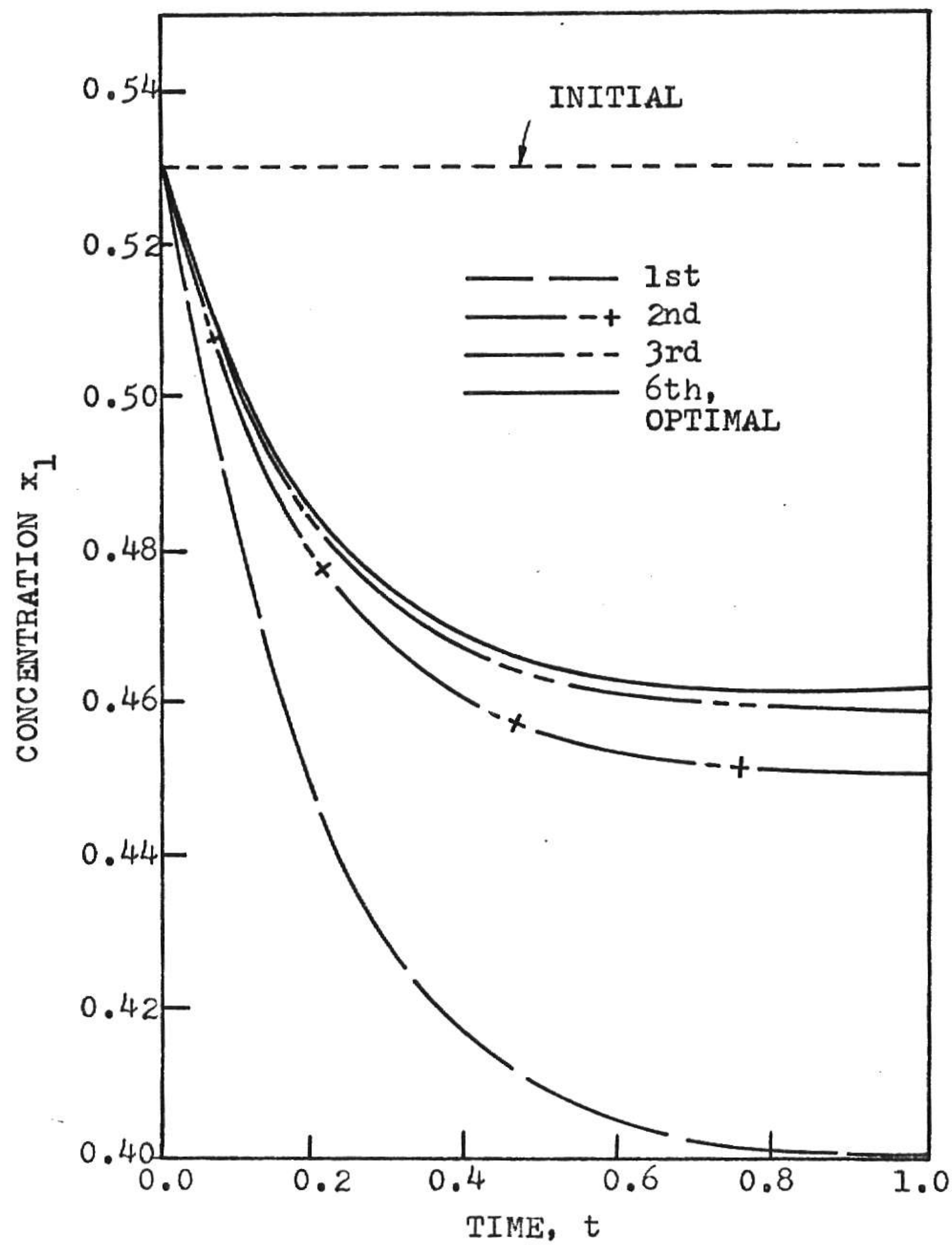

Fig. 13. Convergence Rate of x_1, Problem 1C

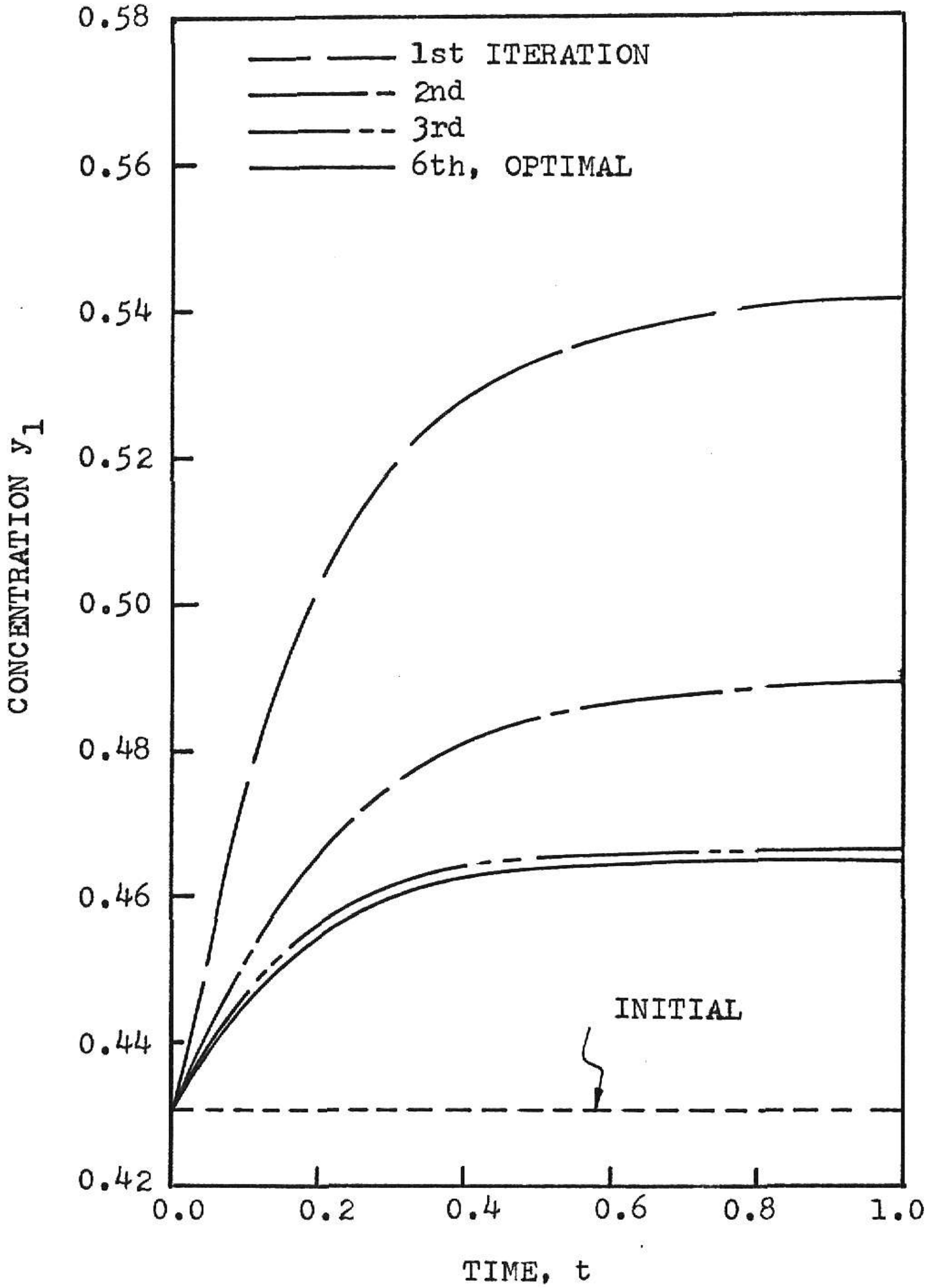

Fig. 14. Convergence Rate of y_1, Problem 1C

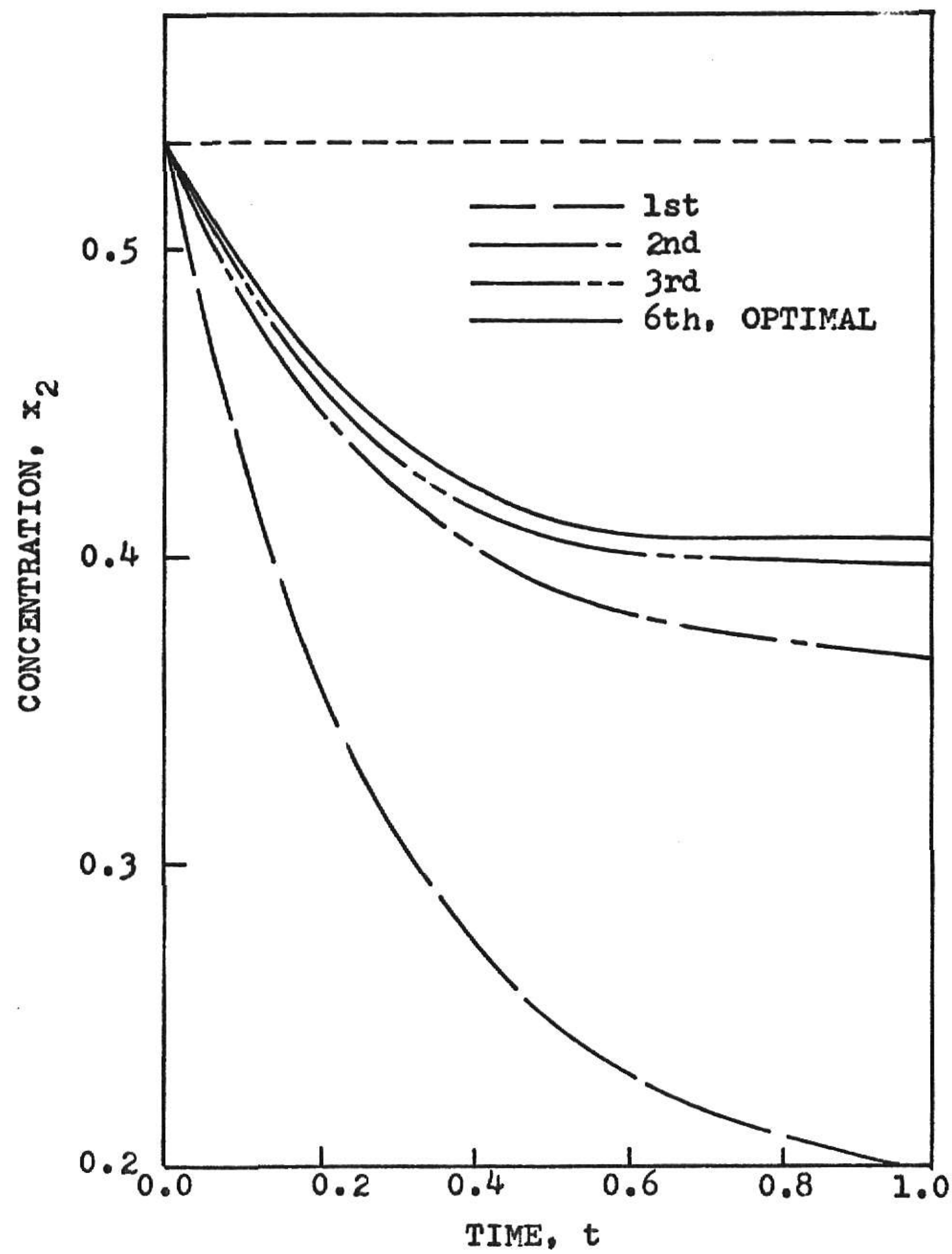

Fig. 15. Convergence Rate of x_2, Problem 1C

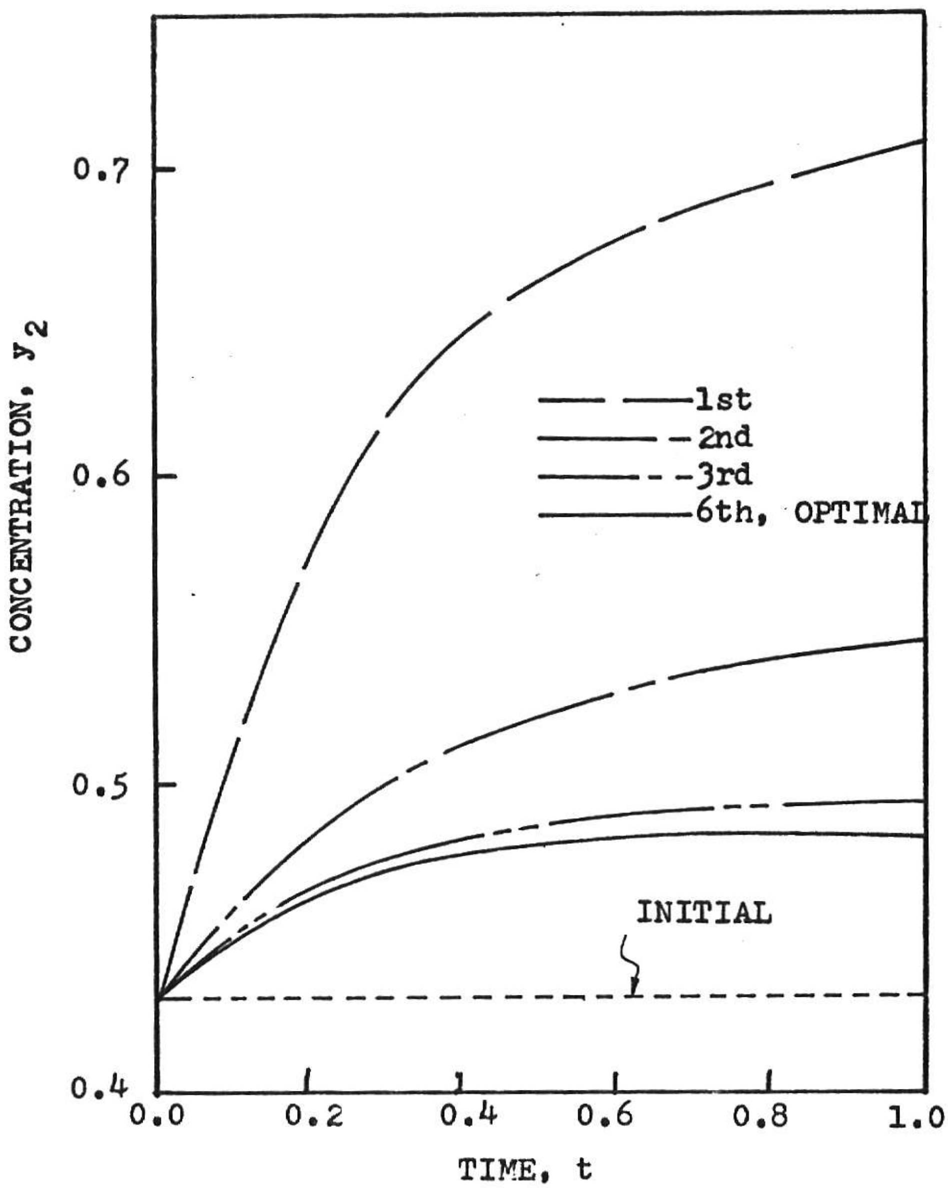

Fig. 16. Convergence Rate of y_2, Problem 1C

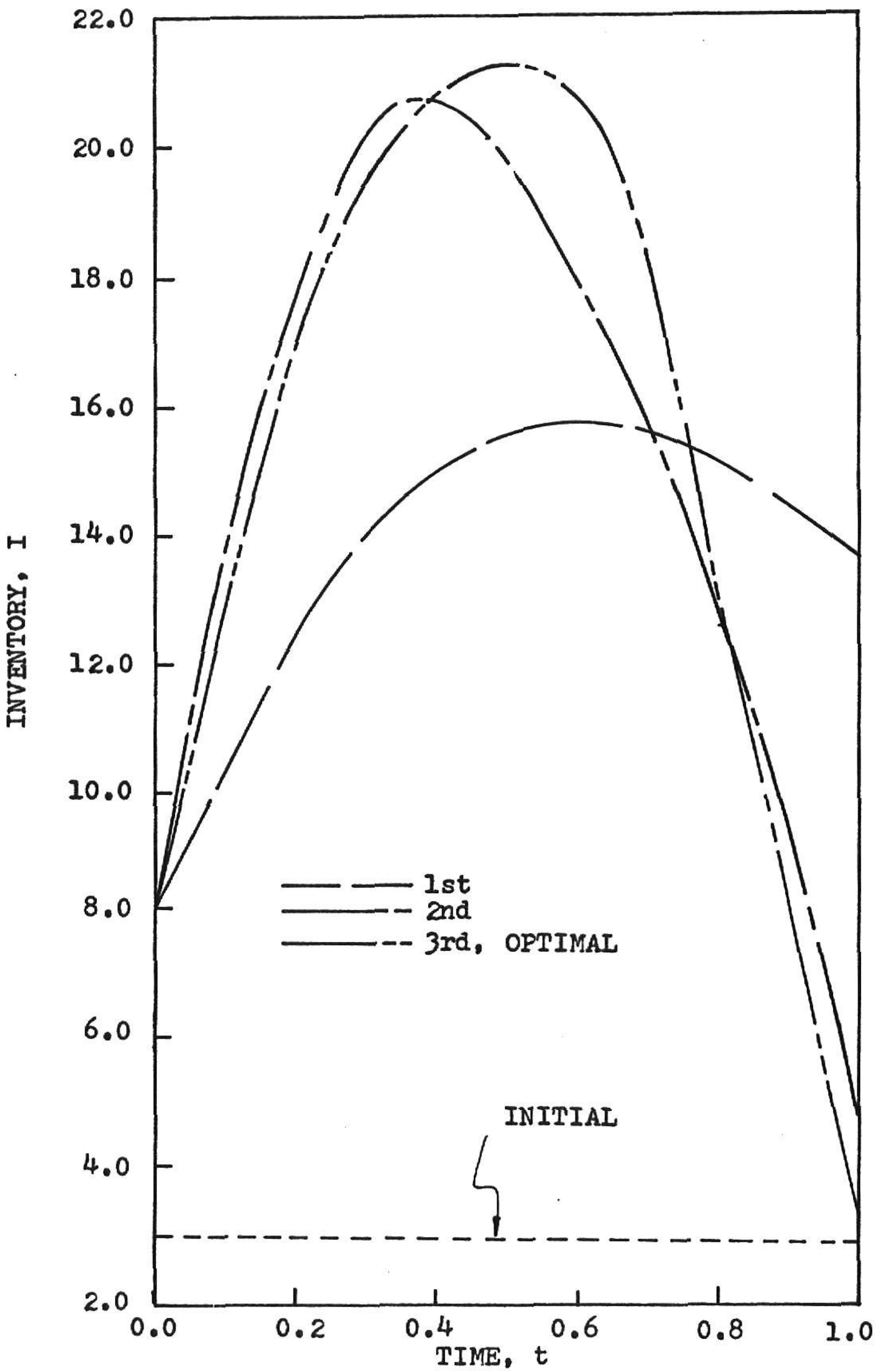

Fig. 17. Convergence Rate of I, Problem 1C

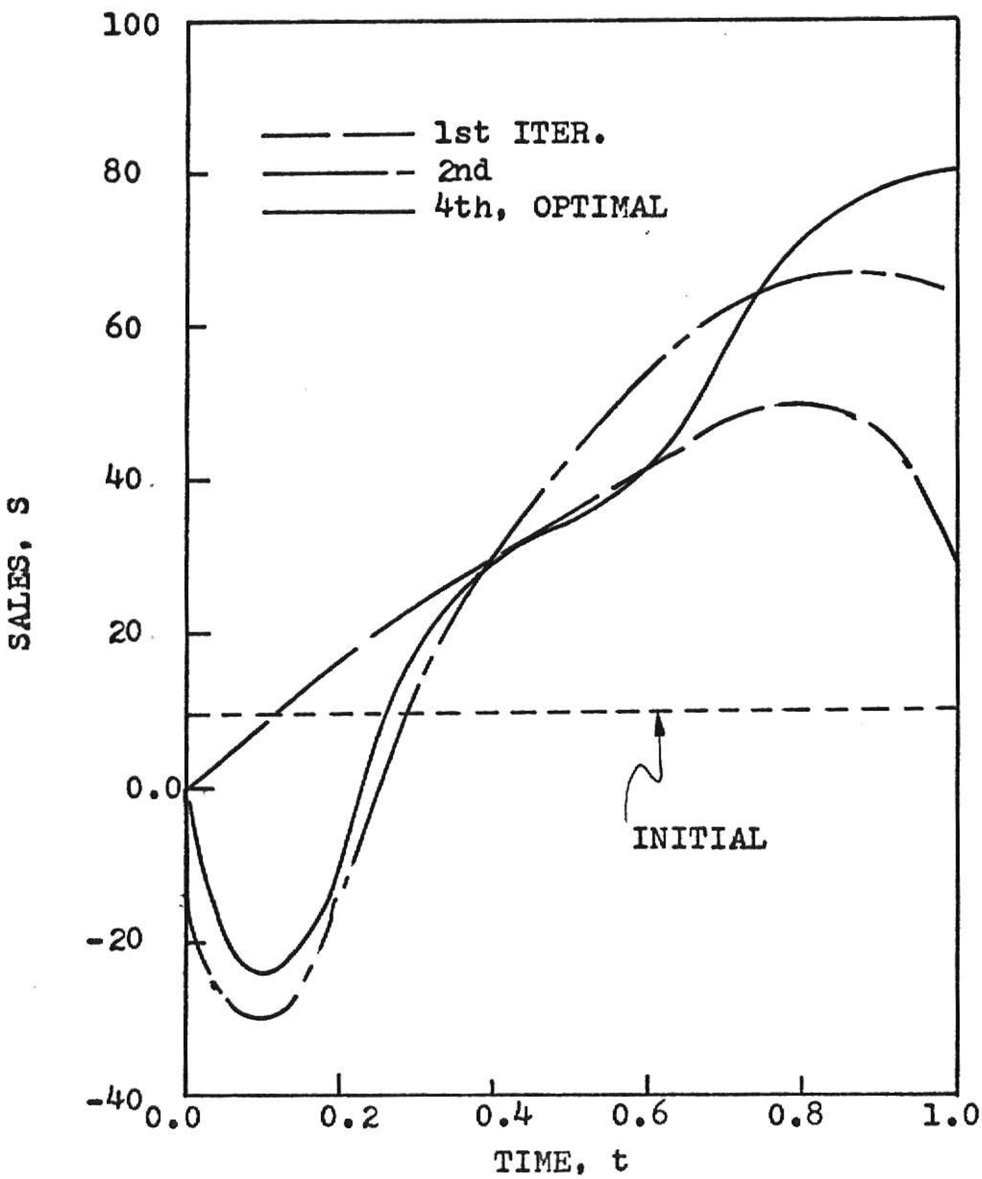

Fig. 18. Convergence Rate of S, Problem 1C

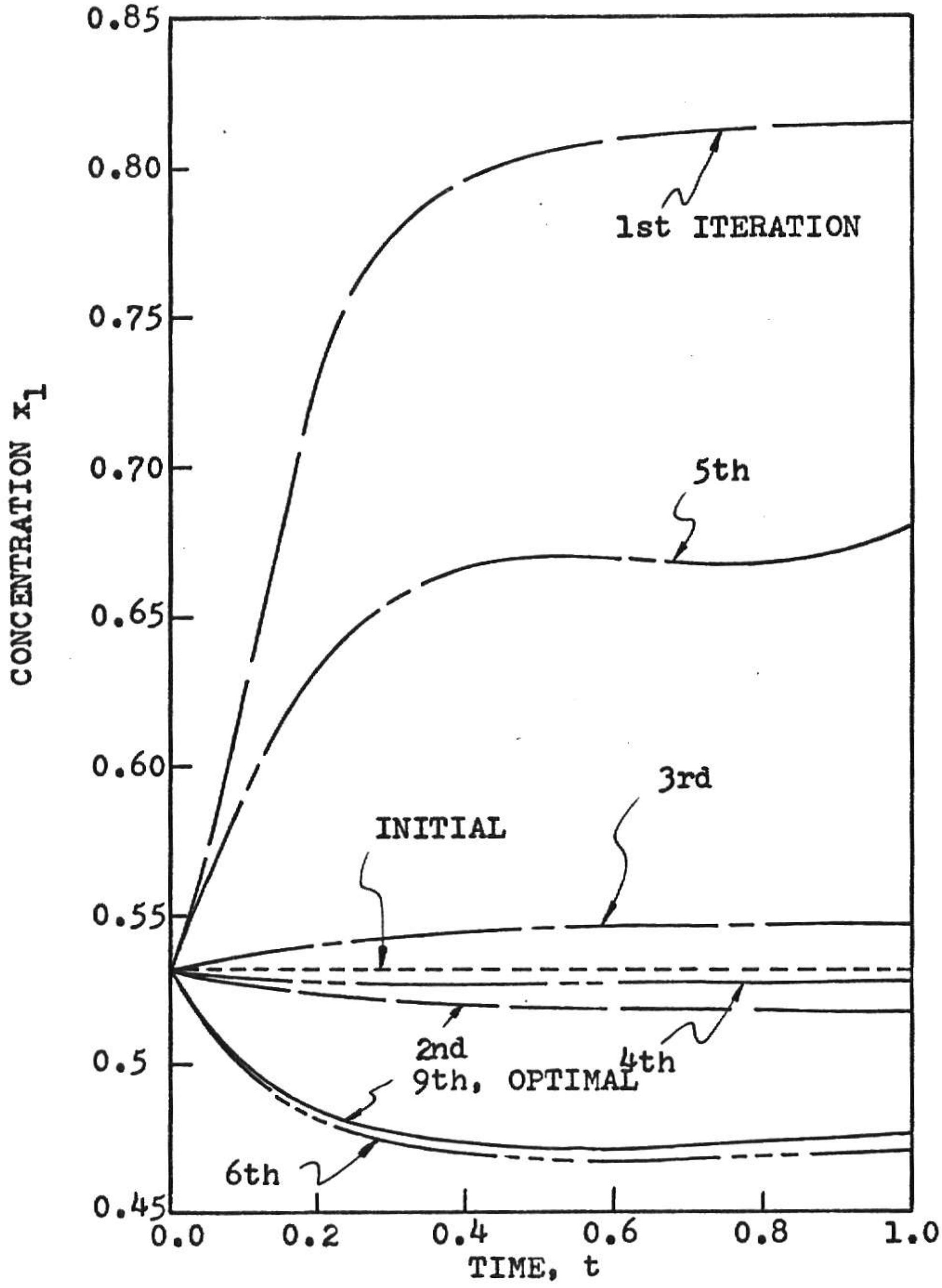

Fig. 19. Convergence Rate of x_1, Problem 3D

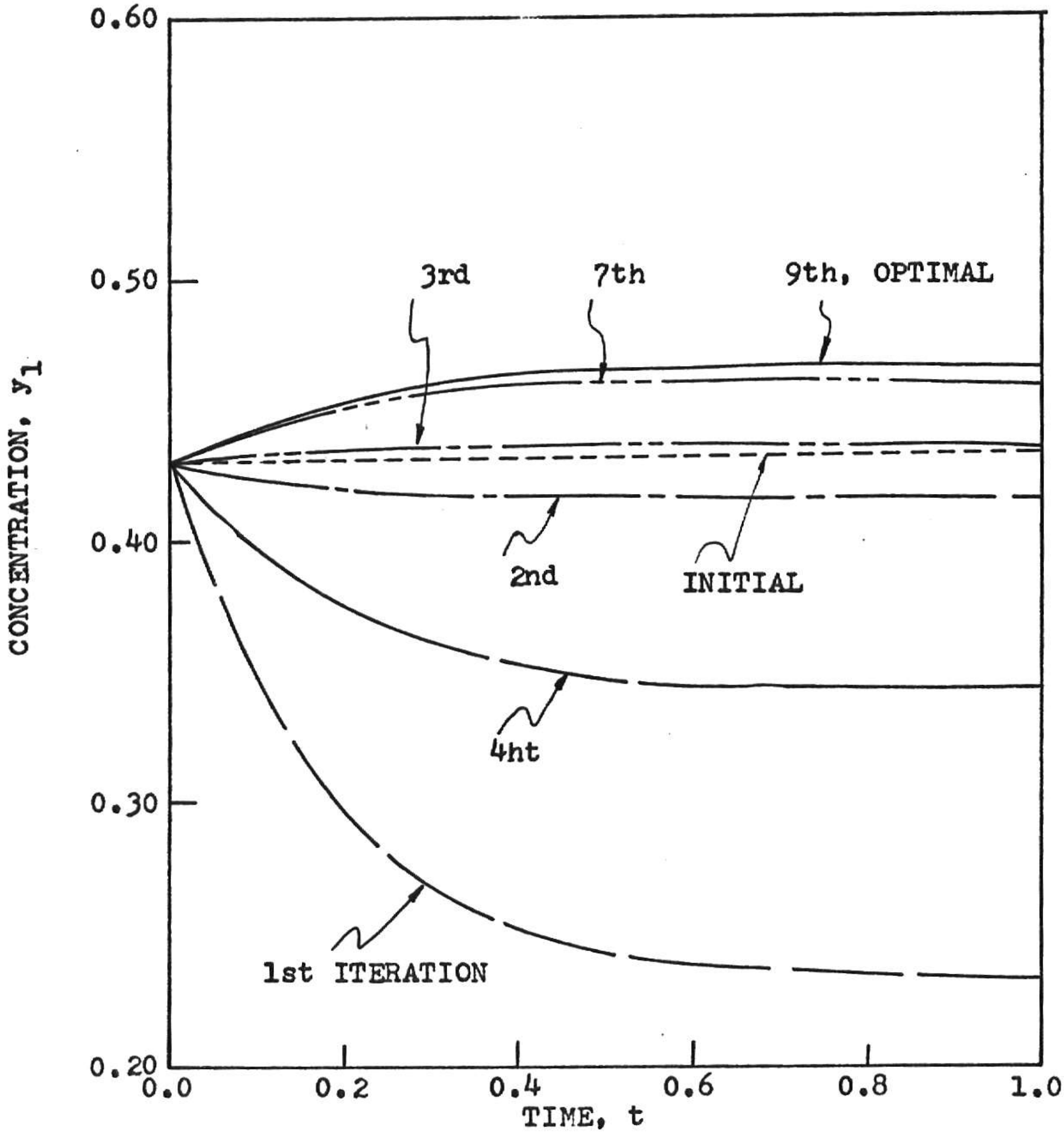

Fig. 20. Convergence Rate of y_1, Problem 3D

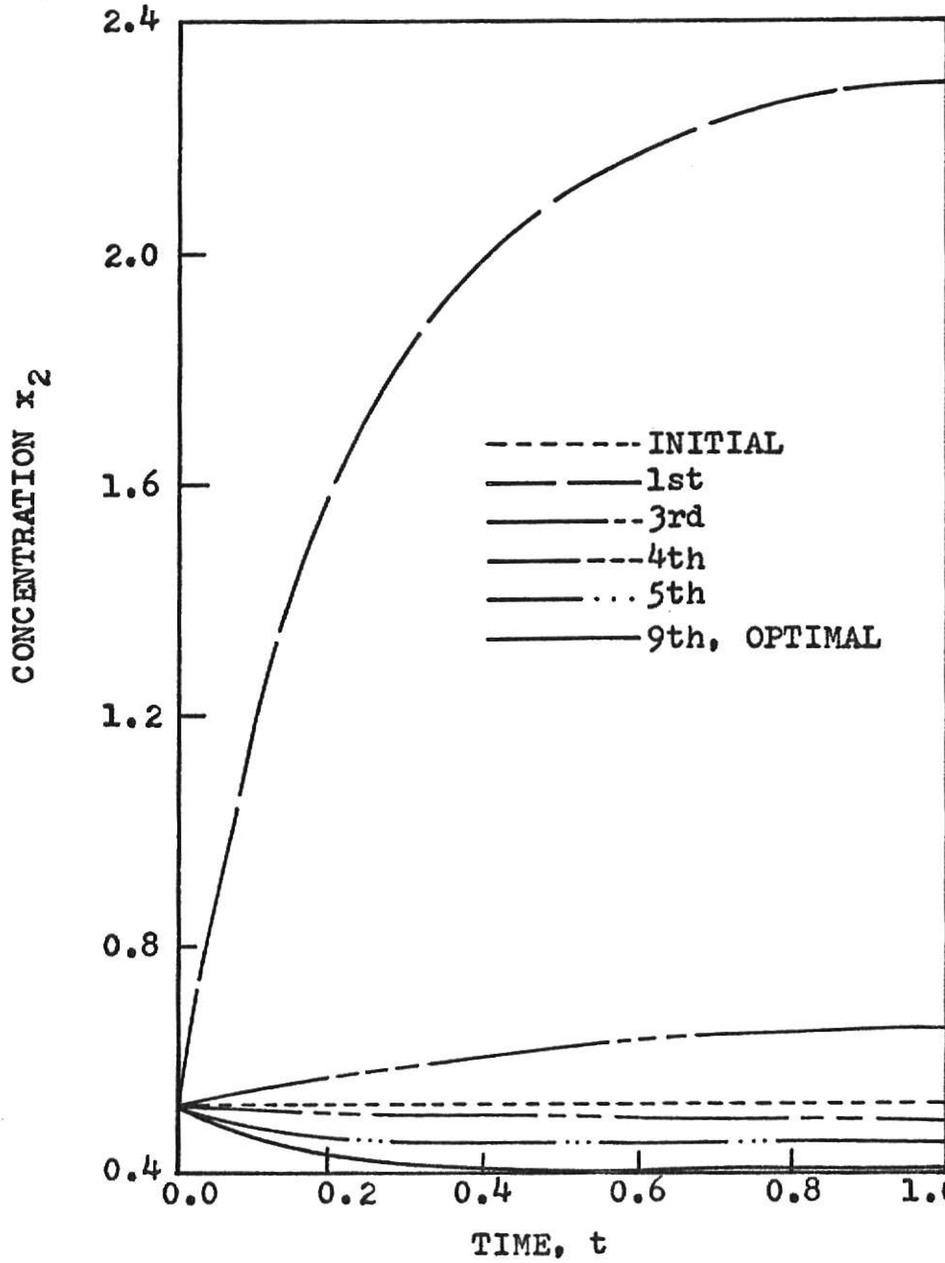

Fig. 21. Convergence Rate of x_2, Problem 3D

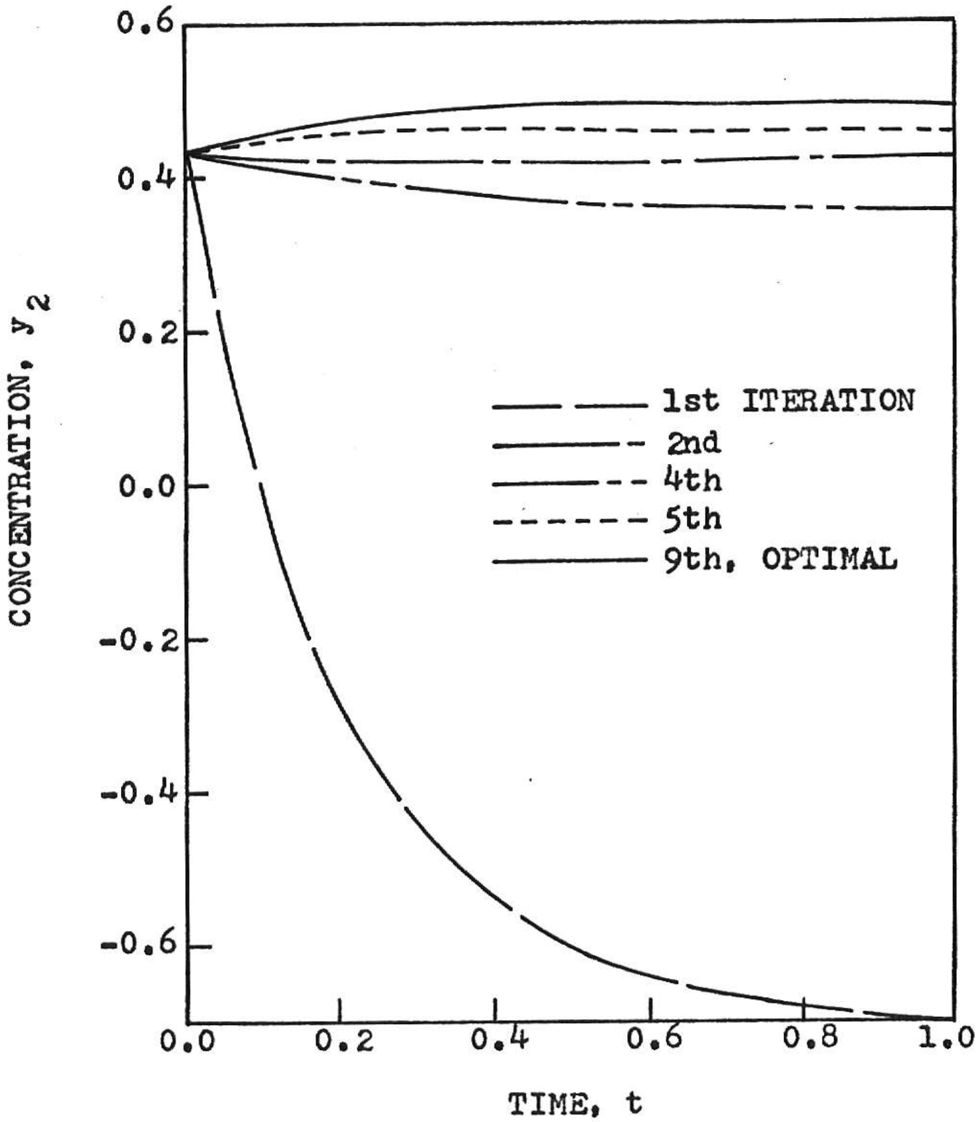

Fig. 22. Convergence Rate of y_2, Problem 3D

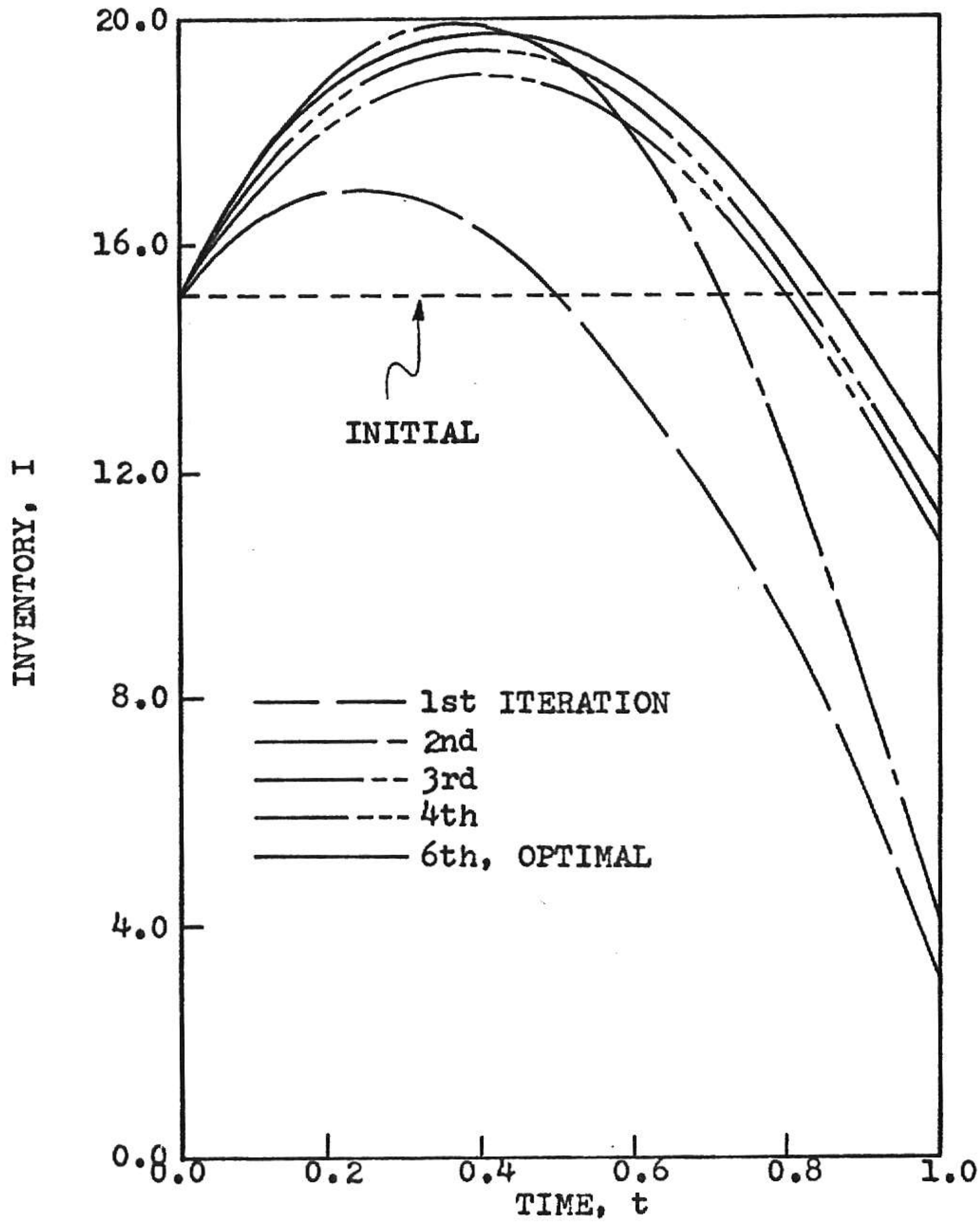

Fig. 23. Convergence Rate of I, Problem 3D

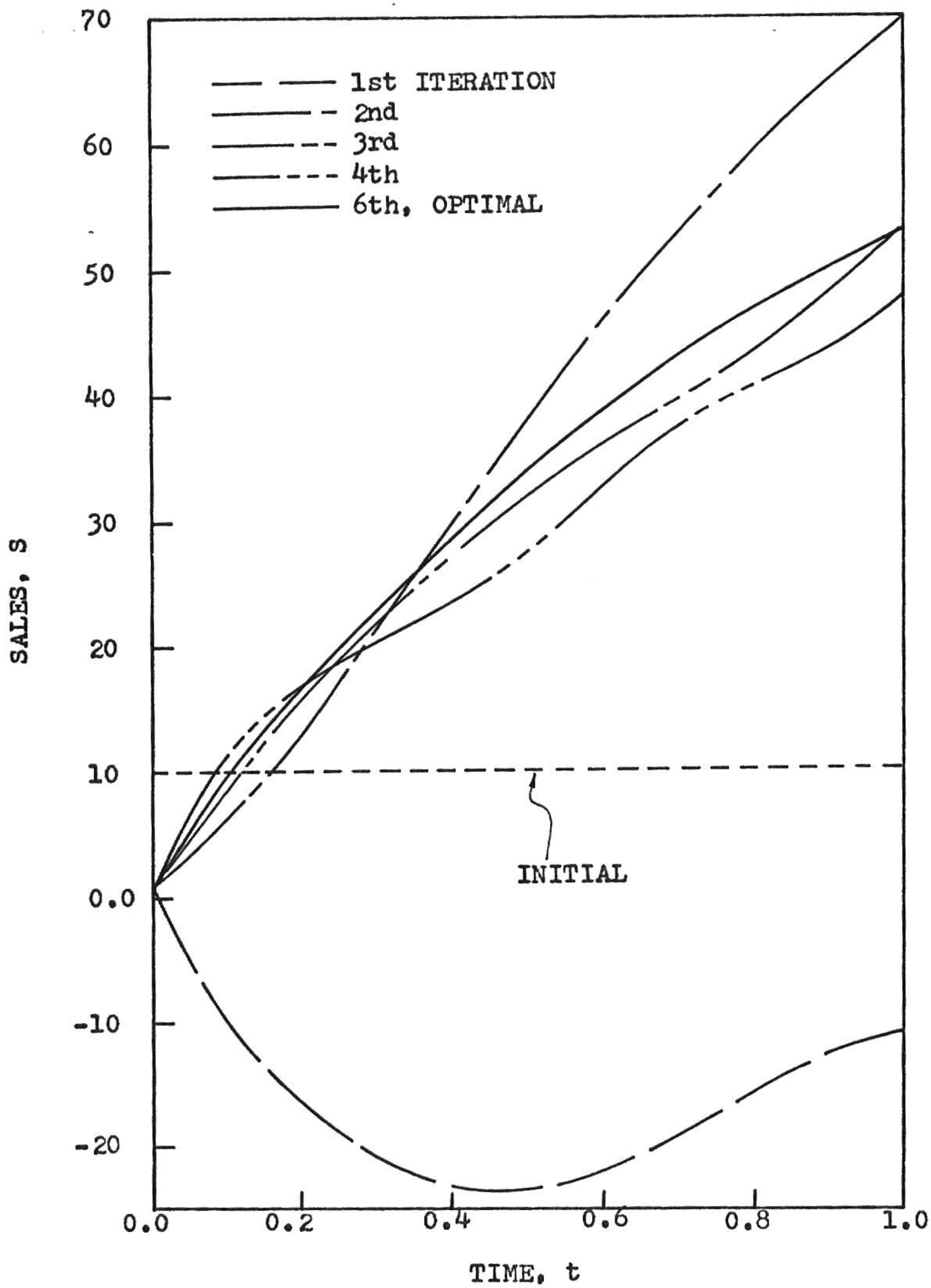

Fig. 24. Convergence Rate of S, Problem 3D

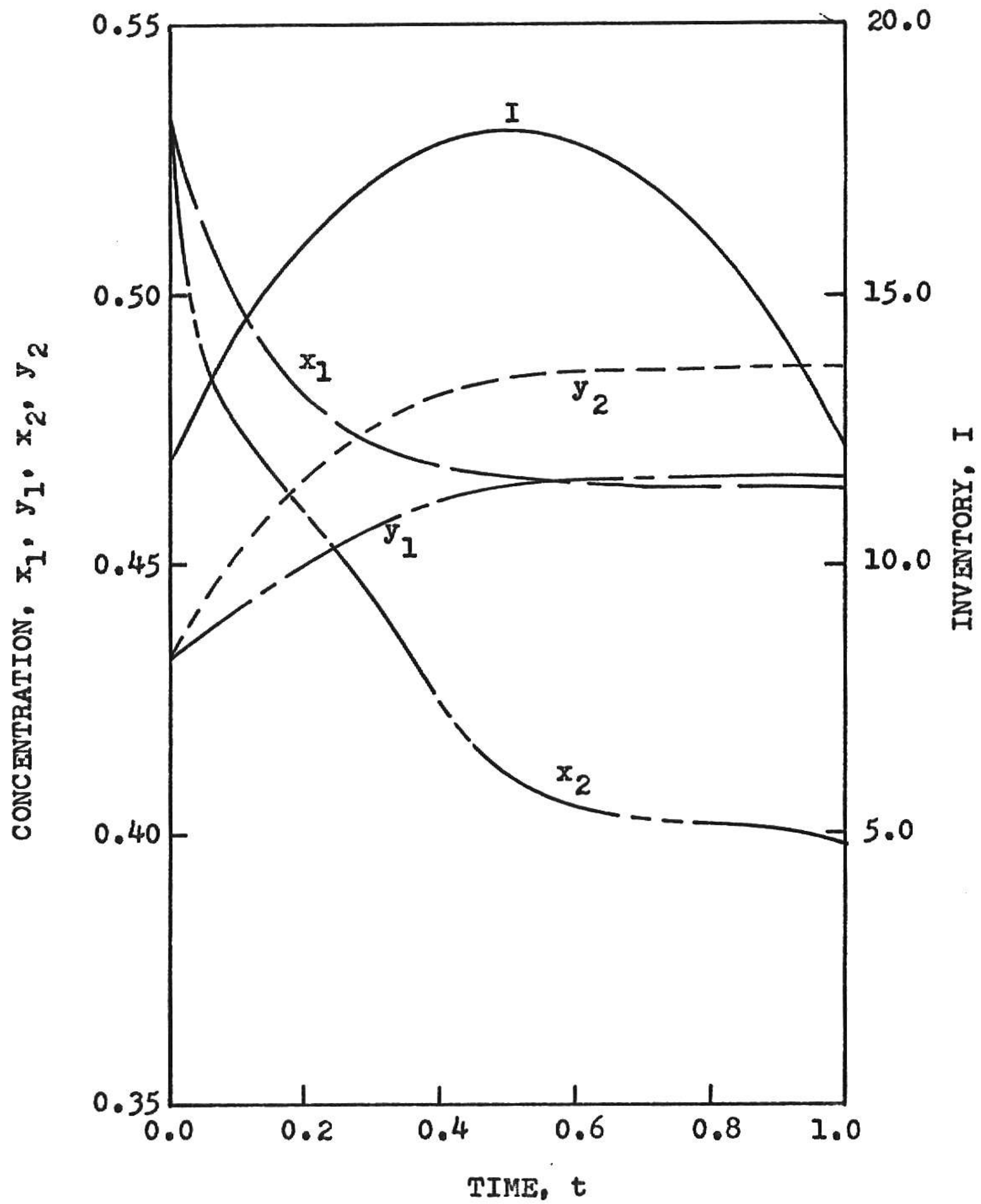

Fig. 25. Optimal Profiles of x_1, y_1, x_2, y_2 and I, Problem 1E

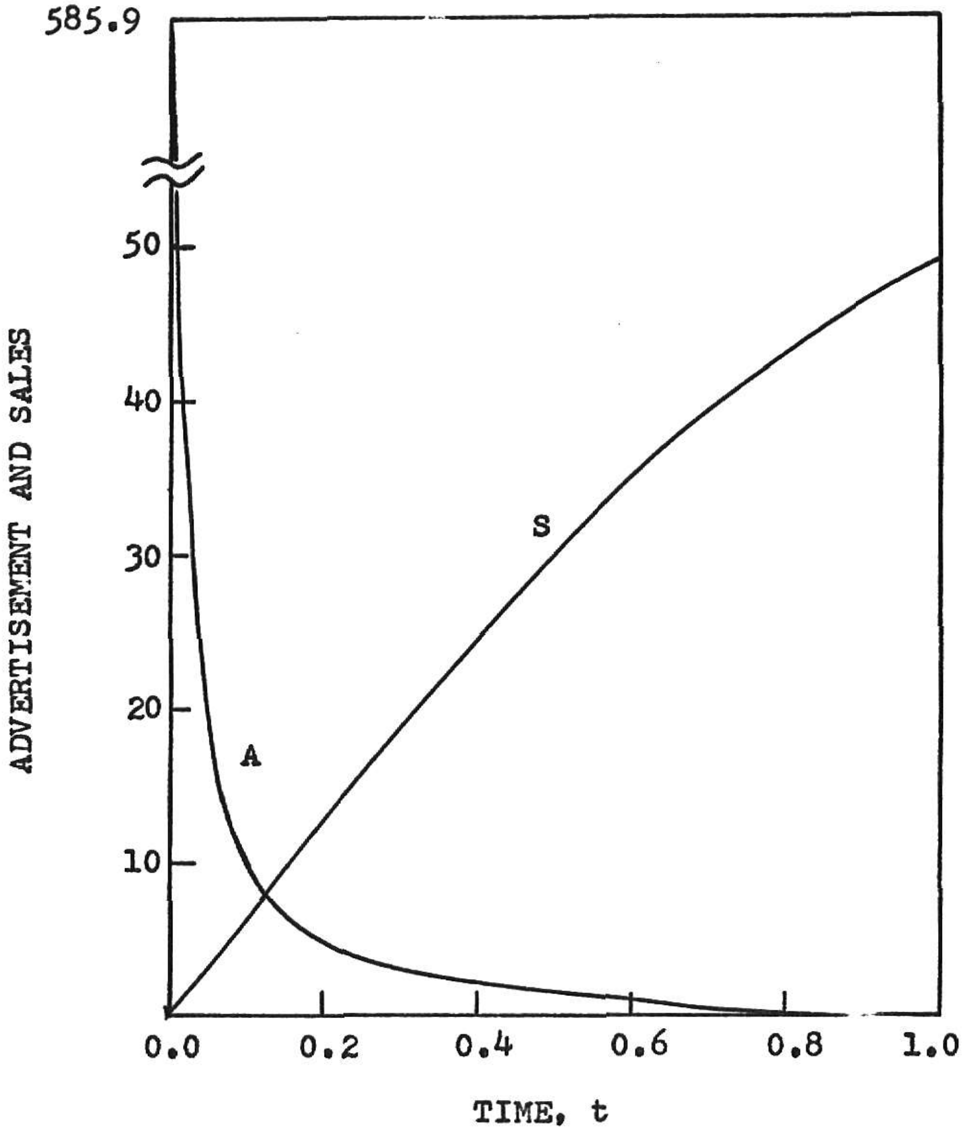

Fig. 26. Optimal Profiles of A and S, Problem 1E

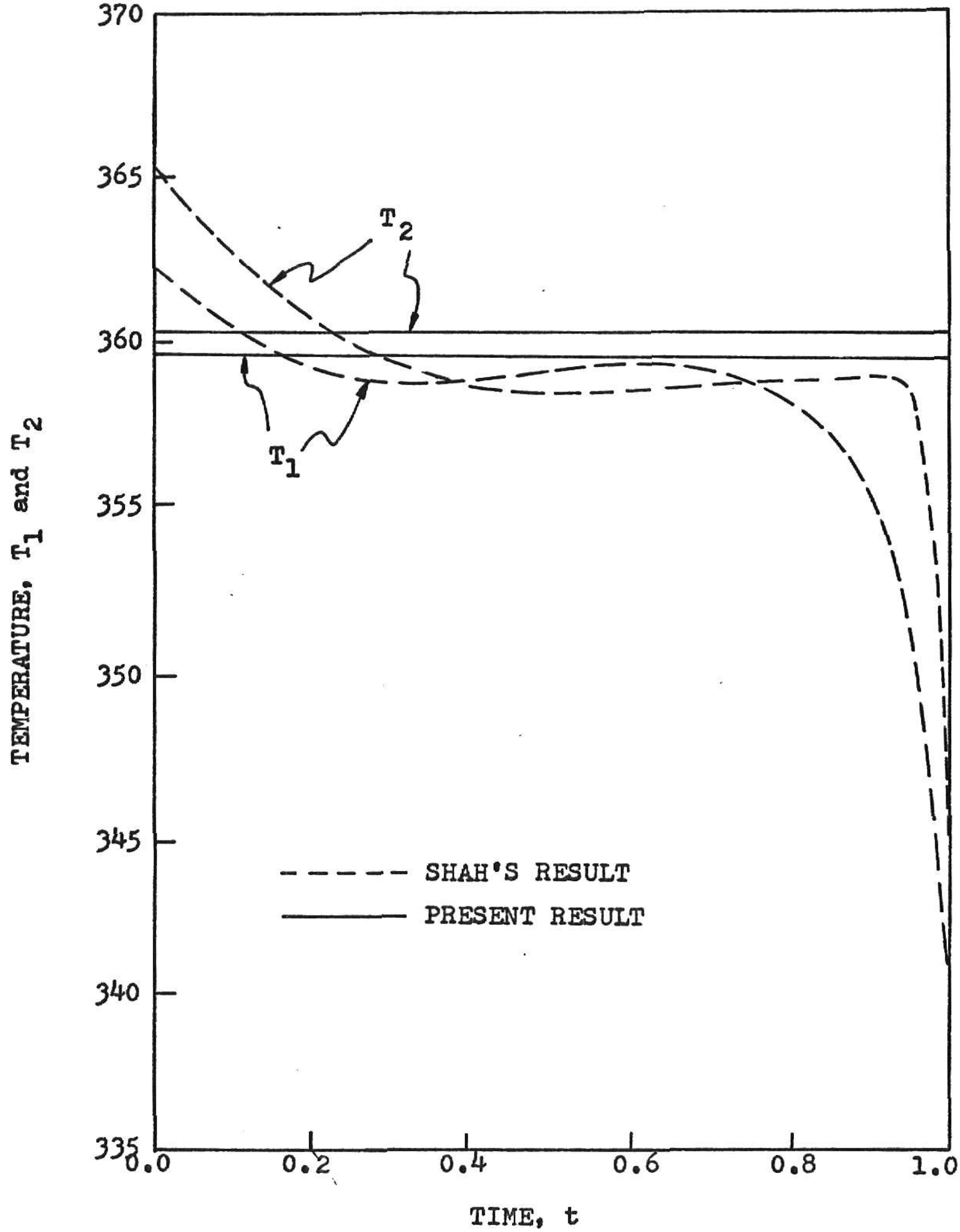

Fig. 27. A Comparison of the Optimal Temperatures in Problem A

CHAPTER 5

A MORE COMPLICATED PRODUCTION PLANNING PROBLEM

In this chapter, a more complicated problem is solved. In addition to the system discussed in Chapter 4, the problem has one more unknow parameter. Before, the volume of the reactor is a fixed constant. But in here, it is considered as an unknown parameter whose optimal value is to be defined.

5-1 DEVELOPMENT OF THE MODEL

The same manufacturing process used in the previous chapter is used here. The only change is having one reactor instead of two.

Because the only change is the number of reactor, the equations remain essentially the same as in Chapter 4 except that Eqs. (4-27) and (4-28) for reactor 2 should be eliminated.

Now the system is represented by the equations

$$V_1 \frac{dx_1}{dt} = q(x_0 - x_1) - V_1 G_a e^{-\frac{E_a}{RT_1}} x_1 \tag{5-1}$$

$$V_1 \frac{dy_1}{dt} = q(y_0 - y_1) - V_1 G_b e^{-\frac{E_b}{RT_1}} y_1 + V_1 G_a e^{-\frac{E_a}{RT_1}} x_1 \tag{5-2}$$

$$\frac{dI}{dt} = q\, y_2 - S \tag{5-3}$$

$$\frac{dS}{dt} = S(C_c + A)(1 - \frac{S}{N}) \tag{5-4}$$

$$\frac{dT_1}{dt} = 0 \tag{5-5}$$

with the boundary conditions

$$x_1(t_0) = x_1^0 \qquad y_1(t_0) = y_1^0 \tag{5-6}$$

$$I(t_0) = I^0 \qquad S(t_0) = S^0 \tag{5-7}$$

In Chapter 4, we considered temperature as a constant parameter. In this chapter, we shall also consider the volume of the reactor as a constant parameter. This can be done, as before, by considering V_1 as additional state variable. Since it is a constant parameter we have the differential equation

$$\frac{dV_1}{dt} = 0 \tag{5-8}$$

In addition to this, a cost function for the reactor must also be included in the objective function. The following cost function is assumed for the reactor

$$g(V_1) = a_1 + a_2V_1 + a_3V_1^2 \tag{5-9}$$

Now, the objective function becomes

$$J = \int_{t_0}^{t_f} [C_1 C_q S + C_2 q\, x_1 + C_3 q(1 - x_1 - y_1) - C_I(I_m - I)^2 - C_A A^2 S^2]\, dt - C_T [T_{1m} - T_1(0)]^2 - g(V_1) \qquad (5\text{-}10)$$

5-2 DEFINITION OF THE PROBLEM

Find the values of $A(t)$, T_1 and V_1 such that the following function is maximized

$$J = \int_{t_0}^{t_f} [C_1 C_q S + C_2 q x_1 + C_3 q(1 - x_1 - y_1) - C_I(I_m - I)^2 - C_A A^2 S^2]\, dt - C_T [T_{1m} - T_1(0)]^2 - g(V_1) \qquad (5\text{-}11)$$

subject to the constraints of

$$\dot{x}_1 = \frac{q}{V_1}(x_0 - x_1) - G_a e^{-\frac{E_a}{RT_1}} x_1 \qquad (5\text{-}12)$$

$$\dot{y}_1 = \frac{q}{V_1}(y_0 - y_1) - G_b e^{-\frac{E_b}{RT_1}} y_1 + G_a e^{-\frac{E_a}{RT_1}} x_1 \qquad (5\text{-}13)$$

$$\dot{I} = q\, y_1 - S \qquad (5\text{-}14)$$

$$\dot{S} = (C_c S + AS)\left[1 - \frac{S}{N}\right] \qquad (5\text{-}15)$$

$$\dot{T}_1 = 0 \qquad (5\text{-}16)$$

$$\dot{V}_1 = 0 \tag{5-17}$$

with the initial conditions

$$\begin{aligned} x_1(t_0) &= x_1^0 \qquad & y_1(t_0) &= y_1^0 \\ I(t_0) &= I^0 \qquad & S(t_0) &= S^0 \end{aligned} \tag{5-18}$$

5-3 FORMULATION OF THE PROBLEM

This problem can also be solved by the calculus of variations. The procedure for obtaining the solution remains essentially the same.

Introduce the Lagrange multipliers, λ_i, $i = 1, 2, \ldots, 6$, and constant multipliers, θ_j, $j = 1, 2, \ldots, 4$, and define the following functions

$$\begin{aligned} F = [\lambda_1(\dot{x}_1 &- \frac{q}{V_1}(x_0 - x_1) + G_a e^{-\frac{E_a}{RT_1}} x_1) \\ &+ \lambda_2(\dot{y}_1 - \frac{q}{V_1}(y_0 - y_1) + G_b e^{-\frac{E_b}{RT_1}} y_1 - G_a e^{-\frac{E_a}{RT_1}} x_1) \\ &+ \lambda_3(\dot{I} - q\, y_1 + S\,) \\ &+ \lambda_4(\dot{S} - C_c S - AS + \frac{C_c S^2}{N} \quad \frac{AS^2}{N}) \\ &+ \lambda_5(\dot{T}_1) \\ &+ \lambda_6(\dot{V}_1) \end{aligned}$$

$$+ C_1C_qS + C_2qx_1 + C_3q(1 - x_1 - y_1) - C_I(I_m - I)^2$$

$$- C_AA^2S^2] \tag{5-19}$$

and

$$G = [\theta_1(x_1(t_0) - x_1^0) + \theta_2(y_1(t_0) - y_1^0) + \theta_3(I(t_0) - I^0)$$

$$+ \theta_4(S(t_0) - S^0)] - C_T[T_{1m} - T_1(0)]^2 - g(V_1) \tag{5-20}$$

Applying the Euler-Lagrange equations, the following Lagrange equations are obtained

$$\frac{d\lambda_1}{dt} = \lambda_1\frac{q}{V_1} + (\lambda_1 - \lambda_2)\, G_a e^{-\frac{E_a}{RT_1}} + q(C_2 - C_3) \tag{5-21}$$

$$\frac{d\lambda_2}{dt} = \lambda_2\,\frac{q}{V_1} + \lambda_2 G_b e^{-\frac{E_b}{RT_1}} - \lambda_5 q - C_3 q \tag{5-22}$$

$$\frac{d\lambda_3}{dt} = 2\, C_I(I_m - I) \tag{5-23}$$

$$\frac{d\lambda_4}{dt} = C_1C_q + \lambda_3 - C_c\lambda_4 - A\lambda_4 + \frac{2C_cS\lambda_4}{N}$$

$$+ \frac{2AS\lambda_4}{N} - 2\, C_AA^2S \tag{5-24}$$

$$\frac{d\lambda_5}{dt} = (\lambda_1 - \lambda_2)G_a e^{-\frac{E_a}{RT_1}}\left(\frac{E_a}{RT_1^2}\right)x_1 + \lambda_2 G_b e^{-\frac{E_b}{RT_1}}\left(\frac{E_b}{RT_1^2}\right)y_1 \tag{5-25}$$

$$\frac{d\lambda_6}{dt} = \frac{\lambda_1 q}{V_1^2}(x_0 - x_1) + \frac{\lambda_2 q}{V_1^2}(y_0 - y_1) \tag{5-26}$$

Using Eq. (2-8) $\frac{\partial F}{\partial u} = 0$, we have

$$A = \frac{\lambda_4}{2C_A}\left(\frac{1}{N} - \frac{1}{S}\right) \tag{5-27}$$

Eliminating the A's in Eqs. (15) and (24), we get

$$\frac{dS}{dt} = C_c S - \frac{C_c S^2}{N} + \frac{S\lambda_4}{C_A N} - \frac{\lambda_4}{2C_A} - \frac{S^2\lambda_4}{2C_A N^2} \tag{5-28}$$

$$\frac{d\lambda_4}{dt} = C_1 C_q + \lambda_3 - C_c\lambda_4 - \frac{\lambda_4^2}{2C_A N} + \frac{2C_c S\lambda_4}{N} + \frac{S\lambda_4^2}{2C_A N^2} \tag{5-29}$$

Now the Equations (12), (13), (14), (16), (17), (21), (22), (23), (25), (26), (28) and (29) represent the system. For these 12 differential equations, only 4 conditions are given. Again the transversality condition is used to obtain the other 8 conditions.

At $t = t_0$, using

$$\frac{G}{T_1(0)} - \frac{F}{T_1} = 0 \quad \text{and} \quad \frac{G}{V_1(0)} - \frac{F}{V_1(0)} = 0$$

we have

$$2\,C_T\left[T_{1m} - T_1(0)\right] = \lambda_5(0)$$

$$-\left[a_2 + 2a_3 V_1(0)\right] = \lambda_4(0) \tag{5-30}$$

At $t = t_f$

$$\lambda_1(t_f) = 0 \qquad \lambda_4(t_f) = 0$$

$$\lambda_2(t_f) = 0 \qquad \lambda_5(t_f) = 0$$

$$\lambda_3(t_f) = 0 \qquad \lambda_6(t_f) = 0 \tag{5-31}$$

Eqs. (30) and (31) give 8 conditions. As a results, we have 12 differential equations with 12 boundary conditions.

5-4 QUASILINEARIZATION

Once again, let us define $\overline{Z}$ as a vector which has components x_1, y_1, I, S, T_1, V_1, λ_1, λ_2, λ_3, λ_4, λ_5, and λ_6, and $\overline{f}$ as the vector function which has the corresponding differential equations as its components.

The 12 equations can be written as

$$\frac{d\overline{Z}}{dt} = \overline{f}(\overline{Z}, t) \tag{5-32}$$

The linearized form of Eq. (32) written in the recurrence relation is

$$\frac{d\overline{Z}_{n+1}}{dt} = \overline{f}_n + J(\overline{Z}_n)\left[\overline{Z}_{n+1} - \overline{Z}_n\right] \tag{5-33}$$

The elements of the Jacobi matrix $J(\overline{Z}_n)$ are listed in the following

$$\frac{\partial f_1}{\partial Z_1} = \frac{-q}{V_1} - G_a \exp(\frac{-E_a}{RZ_5})$$

$$\frac{\partial f_1}{\partial Z_5} = -Z_1 G_a \exp(\frac{-E_a}{RZ_5})(\frac{E_a}{RZ_5^2})$$

$$\frac{\partial f_1}{\partial Z_6} = -q(x_0 - Z_1)/Z_6^2$$

$$\frac{\partial f_2}{\partial Z_1} = G_a \exp(\frac{-E_a}{RZ_5})$$

$$\frac{\partial f_2}{\partial Z_2} = \frac{-q}{Z_6} - G_b \exp(\frac{-E_b}{RZ_5})$$

$$\frac{\partial f_2}{\partial Z_5} = -Z_2 G_b \exp(\frac{-E_b}{RZ_5})(\frac{E_b}{RZ_5^2}) + Z_1 G_a \exp(\frac{-E_a}{RZ_5})(\frac{E_a}{RZ_5^2})$$

$$\frac{\partial f_2}{\partial Z_6} = -q(y_0 - Z_2)/Z_6^2$$

$$\frac{\partial f_3}{\partial Z_2} = q$$

$$\frac{\partial f_3}{\partial Z_4} = -1$$

$$\frac{\partial f_4}{\partial Z_4} = C_c - \frac{2Z_4 C_c}{N} + \frac{Z_{10}}{C_A N} - \frac{Z_4 Z_{10}}{C_A N^2}$$

$$\frac{\partial f_4}{\partial Z_{10}} = \frac{Z_4}{C_A N} - \frac{1}{2C_A} - \frac{Z_4^2}{2C_A N^2}$$

$$\frac{\partial f_7}{\partial Z_5} = (Z_7 - Z_8) G_a \exp(\frac{-E_a}{RZ_5})(\frac{E_a}{RZ_5^2})$$

$$\frac{\partial f_7}{\partial Z_6} = \frac{-Z_7 q}{Z_6^2}$$

$$\frac{\partial f_7}{\partial Z_7} = \frac{q}{Z_6} + G_a \exp\left(\frac{-E_a}{RZ_5}\right)$$

$$\frac{\partial f_7}{\partial Z_8} = - G_a \exp\left(\frac{-E_a}{RZ_5}\right)$$

$$\frac{\partial f_8}{\partial Z_5} = Z_8 \; G_b \exp\left(\frac{-E_b}{RZ_5}\right)\left(\frac{E_b}{RZ_5^2}\right)$$

$$\frac{\partial f_8}{\partial Z_6} = \frac{-Z_8 \; q}{Z_6^2}$$

$$\frac{\partial f_8}{\partial Z_8} = \frac{q}{Z_6} + G_b \exp\left(\frac{-E_b}{RZ_5}\right)$$

$$\frac{\partial f_8}{\partial Z_9} = - q$$

$$\frac{\partial f_9}{\partial Z_3} = - 2C_I$$

$$\frac{\partial f_{10}}{\partial Z_4} = \frac{2C_c Z_{10}}{N} + \frac{Z_{10}^2}{2C_A N^2}$$

$$\frac{\partial f_{10}}{\partial Z_9} = 1$$

$$\frac{\partial f_{10}}{\partial Z_{10}} = -C_c - \frac{Z_{10}}{C_A N} + \frac{2C_c Z_4}{N} + \frac{Z_4 Z_{10}}{C_A N^2}$$

$$\frac{\partial f_{11}}{\partial Z_1} = (Z_7 - Z_8) G_a \exp\left(\frac{-E_a}{RZ_5}\right)\left(\frac{E_a}{RZ_5^2}\right)$$

$$\frac{\partial f_{11}}{\partial Z_2} = Z_8 \; G_b \exp\left(\frac{-E_b}{RZ_5}\right)\left(\frac{E_b}{RZ_5^2}\right)$$

$$\frac{\partial f_{11}}{\partial Z_5} = (Z_7 - Z_8)Z_1\ G_a\ \exp(\frac{-E_a}{RZ_5})(\frac{E_a}{RZ_5^2})(\frac{-2}{Z_5} + \frac{E_a}{RZ_5^2})$$

$$+ Z_8Z_2\ G_b\ \exp(\frac{-E_b}{RZ_5})(\frac{E_b}{RZ_5^2})(\frac{-2}{Z_5} + \frac{E_b}{RZ_5^2})$$

$$\frac{\partial f_{11}}{\partial Z_7} = Z_1\ G_a\ \exp(\frac{-E_a}{RZ_5})(\frac{E_a}{RZ_5^2})$$

$$\frac{\partial f_{11}}{\partial Z_8} = -Z_1\ G_a\ \exp(\frac{-E_a}{RZ_5})(\frac{E_a}{RZ_5^2}) + Z_2\ G_b\ \exp(\frac{-E_b}{RZ_5})(\frac{E_b}{RZ_5^2})$$

$$\frac{\partial f_{12}}{\partial Z_1} = \frac{-Z_7\ q}{Z_6^2}$$

$$\frac{\partial f_{12}}{\partial Z_2} = \frac{-Z_8\ q}{Z_6^2}$$

$$\frac{\partial f_{12}}{\partial Z_6} = \frac{-2Z_7q(x_0 - Z_1)}{Z_6^3} + \frac{-2Z_8q(y_0 - Z_2)}{Z_6^3}$$

$$\frac{\partial f_{12}}{\partial Z_7} = \frac{q(x_0 - Z_1)}{Z_6^2}$$

$$\frac{\partial f_{12}}{\partial Z_8} = \frac{q(y_0 - Z_2)}{Z_6^2}$$

The elements which do not appeal in the above equations are all equal to zero.

The same procedure used in Chapter 4 for solving these linear equations is used here. Since four initial conditions are given, the general solution can be written as

$$\overline{Z}(t) = \overline{Z}\ (t) + \sum_{n=1}^{8} a_m\overline{Z}_{H,m}(t) \tag{5-34}$$

5-5 NUMERICAL ASPECTS

This problem is divided into 9 problems. The constants and the boundary conditions used in each problem is described as following

Problem A

The following values were assumed for the various parameters

$G_a = 0.535 \times 10^{11}$ per minute	$N = 100$
$G_b = 0.461 \times 10^{18}$ per minute	$C_c = 1$
$E_a = 18000$ cal./mole	$a_1 = 5$
$E_b = 30000$ cal./mole	$a_2 = 0.0$
$R = 2$ cal./mole ^oK	$a_3 = 0.0055667$
$q = 60$ gal./min.	$C_T = 0.001$ \$/^oK
$I_m = 10$ gallons	$C_A = \$\ 0.01$
$T_{1m} = 340\ ^oK$	$C_1 = \$\ 7$
$\Delta t = 0.02$	$C_2 = C_3 = \$\ 0.0$
$x_0(t_0) = 0.53$	$C_q = 1$
$y_0(t_0) = 0.43$	$C_I = 1.0$ \$/gal.

The initial conditions were

$$x_1(0) = 0.53, \quad y_1(0) = 0.43, \quad I(0) = 1.0, \quad S(0) = 0.1$$

The various sets of initial approximations used for this problem are listed in Table 19.

Problem B

This problem is essentially the same as problem A, except the cost function of V_1 is changed. All the parameters remain the same, except that

$$a_3 = 0.0075667$$

Two sets of initial approximations used for this problem are given in Table 20.

Problem C

This problem is the modification of problem B. The only parameter which differs from B is

$$a_3 = 0.0065667$$

The initial approximations used for this problem is given in Table 21.

Problem D

This problem has one more given condition, namely, the final inventory.

In addition to this, the values of two parameters are changed. All the other parameters remain the same as in problem A. The two parameters changed are

$$a_1 = 50$$

and

$$I_m = 15$$

The boundary conditions are

$$x_1(0) = 0.53 \quad y_1(0) = 0.43 \quad I(0) = 1.0 \quad S(0) = 0.1$$

$$I(t_f) = 10$$

Two sets of initial approximations are tried for this problem. They are exactly the same as in problem B.

Problem E

The only difference between this problem and problem D is the initial condition of inventory.

$$I(0) = 7$$

The initial approximations used for this problem are shown in Table 22.

Problem F

In this problem, some of the parameters were changed. For clear understanding, all of them are listed in the following

$G_a = 0.535 \times 10^{11}$ per min.	$N = 100$
$G_b = 0.461 \times 10^{18}$ per min.	$C_c = 1$
$E_a = 18000$ cal./mole	$C_T = 0.0005$ $/°K
$E_b = 30000$ cal./mole	C_A = $.0.01
$R = 2$ cal./mole °K	C_1 = $.7.0
$q = 60$ gal./min.	$C_2 = C_3$ = $.0.0
$I_m = 5$ gal.	$C_q = 1.0$
$T_{1m} = 340$ °K	$C_I = 1.0$ $/gal.
$\Delta T = 0.02$	$x_0 = 0.53$
$a_1 = 5$	$y_0 = 0.43$
$a_2 = 0.0$	
$a_3 = 0.0055667$	

The given conditions are

$$x_1(0) = 0.53 \quad y_1(0) = 0.43 \quad I(0) = 5 \quad S(0) = 0.1$$

The initial approximations used for this problem is given in Table 23.

Problem G

The differences between problems G and F are the values of I_m and I(0), the other numerical values remain the same.

$$I_m = 15, \qquad I(0) = 7$$

Four sets of initial approximation were used for this problem which are given in Table 24.

Problem H

In this problem, the only change is

$$I_m = 8$$

All other parameters are same as used in problem F.

Table 25 shows the initial approximations used for this problem.

5-6 COMPUTATIONAL ASPECTS

Basically, the same procedure used in Chapter 4 is used here. The double precision accuracy and the same limits for temperatures were also used in this problem.

At first, a model which has two reactors were solved. But the problems never did converge. When two reactors are in the system, there is a tendency to have very large volume for one reactor and very small volume for the other. This tendency shows that under this new condition, only one reactor is needed.

Another difficulty encountered when solving this problem is the choice of the cost function for V_1. Too high or too low a cost makes the value of V_1 unreasonable, or even negative. Usually the process tends to make use of a very small reactor and meanwhile to have a high temperature. This situation can cause exponential overflow on the computer. Several different cost functions were tried until the one which gave satisfactory results was found.

After finding all the solutions of the 12 variables, the following approximated formula was used to calculate the total profit.

$$J = \sum_{t=0}^{1} [C_1 C_q S + C_2 q x_1 + C_3 q(1 - x_1 - y_1) - C_I (I_m - I)^2 - C_A A^2 S^2]\, t - C_T [T_{1m} - T_1(0)]^2 - g(V_1) \qquad (5\text{-}35)$$

5-7 RESULTS

The results obtained for all the problems are discussed in the following pages.

Problem A

Except for set 2A, all the other four sets of initial approximations converged to the optimal solution.

Figs. 28 through 32 showed the convergence rate of x_1, y_1, I, S, and A. Fig. 33 and Fig. 34 gave the optimal profiles of the six Lagrange multipliers. The convergence rates of T_1, V_1, $I(t_f)$, $S(t_f)$ and J are given in Table 26. Table 27 gives the convergence rate of A(t).

For problem 2A, the first iteration gave a high temperature. After using the limit to hold down the temperature to 370^o, the other value still remained the same which make the system inconsistent. In second iteration, the value of the Lagrange multipliers became extremely large. In 6th iteration, exponential overflow occured on the computer.

Generally speaking, convergence took place in 6 to 7 iterations with three digits accuracy after the decimal point.

Problem B

Both of the two initial approximations listed in Table 20 did not converge. Apparently the change of a_3 made the system unstable. Negative values were obtained for V_1 which made the concentration of y_1 too high. Once this high value was established, it never lowered down even after ten iterations.

Problem C

Problem C also has the unstability problem which occured in the previous problem. For the four sets of initial approximations, only 3C converged to optimal solution.

The convergence rates of $x_1(t)$, $y_1(t)$, $I(t)$, and $S(t)$ were given in Tables 28 through 31. The convergence rates T_1, V_1, $A(0)$ and J were given in Tables 32.

Although the sets of values used in 2C and 3C are very close to each other, problem 2C did not converge even after 15 iterations. The value of V_1 oscillated between minus and plus values during these iterations. The convergence interval of this problem is very narrow; narrow intervals are also the reason why 1C and 4C did not converge.

Problem D

The same sets of initial approximations used in problem B were used here. Only 1D converged to optimal solution. The optimal profiles were shown in Fig. 35. The convergence rates of T_1, V_1, $S(t_f)$, $A(0)$, and J were given in Table 33.

Since the final inventory is fixed at 10 gallons, the process tried to reduce the amount of sale in the beginning. This situation explains why there was negative advertisement in the beginning.

For problem 2D, a negative value of -67 was obtained for V_1 in the second iteration. This made the value of x_1 has the value of 380 in the 4th iteration which caused overflow on the computer.

Problem E

Among the five sets of initial approximations, 1E and 3E did not converge. For 4E and 5E, convergence was obtained in 6 iterations. Problem 2E took about 15 iterations which is very slow compared with 4E and 5E.

The convergence rate of the state variables in problem 4E were shown in Fig. 36-39. Table 34 and 35 gave the convergence rate of the parameters, profit and A(t).

Apparently, problems 1E and 3E were outside the convergence interval. Problem 2E was very close to the margin of this interval which made the convergence rate slow.

In problem D, the advertisement was negative. After raising I(0) to 7 in this problem, negative advertisement did not exist any more.

Problem F

For this problem, 1F converged to the optimal solution, but 2F did not.

The convergence rate of the state variables in problem 1F are given in Figs. 40-43. Table 36 and 37 showed the convergence rate of T_1, V_1, $I(t_f)$, $S(t_f)$, J and A(0).

Problem 2F encountered the same difficulty which happened to problem 2A.

This problem is also very unstable. One common phenomenon which can be seen in each of the convergence figures is that the optimal solution is very close to the solution obtained in the first iteration. This is simply caused by the unstability of the problem.

Problem G

Only problem 2G converged to the optimal solution. The convergence rates of state variables, parameters, and advertisement are given in Figs. 44 to 47 and Tables 38, 39.

The convergence interval for this problem is very small. Notice that the differences between 1G and 2G are the values of $\lambda_1(t)$ and $\lambda_2(t)$. Since problem 2G converged extremely fast in 4 iterations, the only explanation for the reason that 1G, 3G, and 4G did not converge is the small convergence interval.

Problem H

Out of the five sets of initial approximations, 2H and 5H converged to the optimal solution.

The convergence rate of the state variables, parameters, and advertisement are given in Figs. 48 to 51 and Tables 40, 41.

Generally speaking, for 2H and 5H, convergence was obtained in 6 iterations for three digits accuracy after the decimal point.

For both 1H and 4H, a very high temperature was obtained in the first few iterations. This high temperature droped sharply later on and caused exponential overflow immediately. Problem

3H had a very small value for V_1 in iteration 5 which also immediately caused overflow on the computer.

5-8 DISCUSSION

All the results showed that no severe difficulty existed in this problem. However considering V_1 as an unknown parameter does make the problem more unstable.

Since V_1 appears in Equations (5-12) and (5-13) as the denominator of the first term, the value of V_1 has strong influences over the changing rate of x_1 and y_1. Small or negative values of V_1 usually make the concentrations of x_1 and y_1 unreasonable.

The value of V_1 obtained for all the problems is around 22 gallons which is very close to the sum of reactors 1 and 2 in the previous chapter. These results suggest that having one big reactor is sufficient for the system.

In this problem, a_3 is a critical parameter. Even a small change of this parameter may cause the system to become unstable which can be seen in problems B and C. Another critical value is the initial inventory, I(0). The combination of I(0) and I_m determines the amount of advertising. A large value of I_m and small value of I(0) tend to reduce the sale by having negative advertisement. When the value of I(0) is very close to I_m, the process tends to have large amount of advertisement in the beginning to bring up the sales. It caused negative inventory at the end even when the advertisement is almost equal to zero. This situation can be observed in problem 1F.

The solutions obtained for problems A, C, F, and H have negative inventory. The solution of problem D has negative advertisement. These negative inventory and advertisement are unreasonable in real situations.

The convergence interval of this problem is very small. The two-phase method which Mehrotra [18] has applied to a similar problem may eliminate the convergence difficulty encountered in this problem.

Table 19. Initial Approximations for problem A

Set No.	$x(t)$	$y(t)$	$I_0(t)$	$S_0(t)$	$T_1(t)$	$V_1(t)$	$\lambda_1^{(t)}$	$\lambda_2^{(t)}$	$\lambda_3^{(t)}$	$\lambda_4^{(t)}$	$\lambda_5^{(t)}$	$\lambda_6^{(t)}$
1A*	0.53	0.43	4	4	350	10	-0.5	-20	-5	-1	0	0.1
2A	0.53	0.43	1	1	340	12	-1	-1	-1	-1	-1	-1
3A*	0.53	0.43	2	2	330	15	-1	-10	0	0	0	0
4A*	0.53	0.43	1	1	345	12	-2	-15	-0.5	-0.5	-0.5	-0.5
5A*	0.53	0.43	3	3	355	20	-0.8	-25	-3	-1	0	-0.1

Table 20. Initial Approximations for Problem B and D

Set No.	$x(t)$	$y(t)$	$I_0(t)$	$S(t)$	$T_1(t)$	$V_1(t)$	$\lambda_1^{(t)}$	$\lambda_2^{(t)}$	$\lambda_3^{(t)}$	$\lambda_4^{(t)}$	$\lambda_5^{(t)}$	$\lambda_6^{(t)}$
1B(D*)	0.53	0.43	2	3	330	12	-3	-20	-2	-2	-2	-2
2B(D)	0.53	0.43	5	5	340	10	-10	-10	1	1	1	1

* Converged to optimal solution

Table 21. Initial Approximations for Problem C

Set No.	$x(t)$	$y(t)$	$I(t)$	$S(t)$	$T_1(t)$	$V_1(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$
1C	0.53	0.43	5	5	350	15	-5	-20	-5	-1	0.01	-0.1
2C	0.53	0.43	6	10	340	20	-4	-25	-3	-1	-1	-1
3C*	0.53	0.43	2	3	330	12	-3	-20	-2	-2	-2	-2
4C	0.53	0.43	5	5	340	10	-10	-10	1	1	1	1

Table 22. Initial Approximations for problem E

Set No.	$x(t)$	$y(t)$	$I(t)$	$S(t)$	$T_1(t)$	$V_1(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$
1E	0.53	0.43	7	4	345	15	-7	-15	-3	0.0	0.0	0.0
2E*	0.53	0.43	5	5	340	13	-5	-18	-5	-0.01	0.0	0.0
3E	0.45	0.45	13	13	350	18	-10	-30	-4	-0.7	0.0	-0.1
4E*	0.40	0.50	10	15	345	10	-15	-40	-6	-0.1	0.1	-0.01
5E*	0.45	0.45	13	13	350	18	-20	-60	-4	-0.7	0.0	-0.1

Table 23. Initial Approximations for Problem F

Set No.	x(t)	y(t)	I(t)	S(t)	$T_1(t)$	$V_1(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$
1F*	0.53	0.43	10	20	345	15	-10	-40	-5	-1	0.0	0.0
2F	0.53	0.43	4	30	370	9	4	-5	-0.1	-2	-0.1	-0.1

Table 24. Initial Approximations for problem G

Set No.	x(t)	y(t)	I(t)	S(t)	$T_1(t)$	$V_1(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$
1G	0.53	0.43	4	30	370	9	4	-5	-0.1	-2	-0.1	-0.1
2G*	0.53	0.43	4	30	370	9	-20	-40	-0.1	-2	-0.1	-0.1
3G	0.53	0.43	4	4	340	10	-1	-10	0.0	0.0	0.0	-0.1
4G	0.53	0.43	4	4	340	10	-20	-40	0.0	0.0	0.0	-0.1

Table 25. Initial Approximations for Problem H

Set No.	x(t)	y(t)	I(t)	S(t)	$T_1(t)$	$V_1(t)$	$\lambda_1(t)$	$\lambda_2(t)$	$\lambda_3(t)$	$\lambda_4(t)$	$\lambda_5(t)$	$\lambda_6(t)$
1H	0.45	0.45	6	30	340	10	-10	-15	0.0	-3	-0.2	-0.1
2H*	0.4	0.5	3	20	345	15	-15	-25	-0.1	-4	-1	0.0
3H	0.45	0.45	6	30	340	10	-20	-40	0.0	-3	-0.2	-0.1
4H	0.4	0.5	7	25	330	20	-25	-45	0.0	-2	0.0	0.0
5H*	0.43	0.53	2	10	350	20	-10	-15	-1	-3	0.0	0.0

Table 25.a. Initial values used for particular and homogeneous solution

	P.I. for A,B, C,D	P.I. for E,G	P.I. for F,H	Homogeneous solutions							
				1	2	3	4	5	6	7	8
$x_1(0)$	0.53	0.53	0.53	0	0	0	0	0	0	0	0
$y_1(0)$	0.43	0.43	0.43	0	0	0	0	0	0	0	0
$I(0)$	1.0	7.0	5.0	0	0	0	0	0	0	0	0
$S(0)$	0.1	0.1	0.1	0	0	0	0	0	0	0	0
$T_1(0)$	0	0	0	1	0	0	0	0	0	0	0
$V_1(0)$	0	0	0	0	1	0	0	0	0	0	0
$\lambda_1(0)$	0	0	0	0	0	1	0	0	0	0	0
$\lambda_2(0)$	0	0	0	0	0	0	1	0	0	0	0
$\lambda_3(0)$	0	0	0	0	0	0	0	1	0	0	0
$\lambda_4(0)$	0	0	0	0	0	0	0	0	1	0	0
$\lambda_5(0)$	0	0	0	0	0	0	0	0	0	1	0
$\lambda_6(0)$	0	0	0	0	0	0	0	0	0	0	1

Table 26 Convergence Rates of T_1, V_1, $I(t_f)$, $S(t_f)$, and J, problem 5A

ITER.	0	1	2	3	4	5	6	7
T_1	355.0	403.44	365.84	362.38	360.88	360.44	360.63	360.63
V_1	20.0	35.27	21.68	21.03	20.65	20.60	20.60	20.60
$I(t_f)$	3.0	-1.37	-0.57	-0.75	-0.79	-0.80	-0.80	-0.80
$S(t_f)$	3.0	60.64	53.74	53.20	53.05	53.03	53.03	53.03
J	-	173.41	147.90	145.30	144.54	144.44	144.44	144.44

Table 27 Convergence Rate of A(t), problem 5A

ITER. / TIME	1	2	3	4	5	6	7
0.0	618.98	564.86	539.65	531.60	530.42	530.40	530.40
0.2	4.72	5.04	5.08	5.09	5.10	5.10	5.10
0.4	1.85	2.22	2.24	2.25	2.25	2.25	2.25
0.6	0.87	1.19	1.20	1.21	1.21	1.21	1.21
0.8	0.37	0.56	0.57	0.57	0.57	0.57	0.57
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 28. Convergence Rate of $x_1(t)$, problem 3C

TIME \ ITER	0	1	2	3	4	5	6	7	8	9	10	11	12
0.0	0.33	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53	0.53
0.2	0.53	0.56	0.49	0.28	0.39	-0.42	0.43	-0.06	0.33	0.40	0.47	0.47	0.47
0.4	0.53	0.57	0.39	0.14	0.39	-0.40	0.35	-0.54	0.14	0.21	0.43	0.44	0.44
0.6	0.53	0.57	0.18	0.00	0.41	-0.46	0.28	-0.93	0.05	0.00	0.40	0.43	0.43
0.8	0.53	0.57	-0.22	-0.18	0.42	-0.52	0.23	-1.25	0.01	-0.18	0.39	0.42	0.42
1.0	0.53	0.57	-1.05	-0.30	0.42	-0.54	0.19	-1.51	0.00	-0.33	0.38	0.42	0.42

Table 29. Convergence Rate of $y_1(t)$, Problem 3C

TIME \ ITER	0	1	2	3	4	5	6	7	8	9	10	11	12
0.0	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43	0.43
0.2	0.43	0.40	0.45	0.38	0.37	-0.96	-0.20	0.38	0.63	0.56	0.47	0.46	0.46
0.4	0.43	0.39	0.54	0.34	0.37	-0.95	-0.83	1.22	1.17	0.80	0.51	0.47	0.47
0.6	0.43	0.39	0.72	0.39	0.37	-0.93	-1.07	2.38	1.48	1.03	0.55	0.47	0.47
0.8	0.43	0.38	1.08	0.56	0.35	-0.84	-1.14	3.52	1.51	1.51	0.59	0.46	0.47
1.0	0.43	0.38	1.79	0.59	0.34	-0.71	-1.06	4.43	1.51	1.19	0.61	0.46	0.47

Table 30. Convergence Rate of I(t), Problem 3C

TIME \ ITER	0	1	2	3	4	5	6	7	8	9	10	11	12
0.0	2.0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
0.2	2.0	4.92	4.48	5.11	4.96	-0.52	6.48	2.89	3.37	4.21	5.04	5.15	5.14
0.4	2.0	6.34	5.10	6.16	6.50	-1.74	5.85	0.51	3.96	5.16	6.52	6.90	6.86
0.6	2.0	5.44	4.27	4.68	5.69	-3.14	-2.18	-1.38	8.68	6.34	5.72	6.21	6.18
0.8	2.0	2.74	4.34	2.29	2.70	-6.60	-3.44	1.02	12.33	7.67	3.25	3.43	3.46
1.0	2.0	-0.64	9.09	-0.28	-2.12	-11.14	-9.74	8.21	12.50	8.55	-0.41	-0.96	-0.82

Table 31. Convergence Rate of S(t), Problem 3C

TIME \ ITER	0	1	2	3	4	5	6	7	8	9	10	11	12
0.0	3.00	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
0.2	3.00	10.83	18.05	9.63	8.87	-45.27	-23.97	29.69	38.88	25.52	14.49	12.61	12.60
0.4	3.00	22.60	34.72	22.60	20.57	-53.69	-37.14	87.38	54.26	43.63	29.52	25.75	25.88
0.6	3.00	33.02	47.79	34.91	31.90	-43.68	-41.20	145.17	64.62	55.49	41.90	37.22	37.37
0.8	3.00	39.79	57.04	44.83	41.38	-29.31	-36.72	184.01	80.35	63.48	51.20	46.39	46.51
1.0	3.00	38.98	63.33	51.70	48.09	-19.64	-36.74	231.15	101.45	69.52	57.69	52.91	51.97

Table 32. Convergence Rates of T_1, V_1, A(0), and J, Problem 3C

ITER	0	1	2	3	4	5	6	7	8	9	10	11	12
T_1	330.0	242.2	406.9	383.5	384.6	546.2	376.1	404.9	375.6	367.3	360.6	361.0	360.7
V_1	12.0	-17.5	-45.4	7.50	6.4	-15.4	-31.2	-42.9	-80.5	71.5	23.5	19.3	19.1
A(0)	-	416.2	833.3	279.2	266.7	-3404.8	-1569.7	608.9	2399.7	1413.6	596.2	522.9	527.6
J	-	98.14	176.7	128.3	112.3	-746.5	-391.5	684.3	231.4	195.2	166.6	143.2	144.0

Table 33. Convergence Rates of T_1, V_1, $S(t_f)$, $A(0)$, and J, Problem D

ITER.	0	1	2	3	4	5	6	7
T_1	330.00	221.38	435.18	382.61	382.69	398.31	411.82	354.62
V_1	12.00	-26.54	-44.75	-40.35	-68.02	-57.89	-54.64	-93.99
$S(t_f)$	3.00	25.23	46.61	33.75	7.43	-16.55	38.70	92.91
A(0)	-	-198.37	-26.78	-324.40	-734.83	-1329.64	-1206.60	-184.61
J	-	-31.98	25.13	-14.42	-136.90	-275.99	-132.74	16.67

Table 33. Convergence Rates of T_1, V_1, $S(t_f)$, $A(0)$, and J, Problem D (Cont'd)

ITER.	8	9	10	11	12	13	14
T_1	355.80	356.78	349.16	364.35	361.73	360.51	360.41
V_1	-23.59	-46.74	39.21	28.19	21.83	22.78	22.77
$S(t_f)$	50.33	45.59	51.36	39.57	39.39	39.36	39.34
A(0)	-355.85	-16.38	127.51	-115.64	-84.46	-85.24	-85.81
J	48.10	37.27	54.21	25.70	25.58	25.12	25.04

Table 34 Convergence Rates of T_1, V_1, $S(t_f)$, and J, problem 4E

ITER.	0	1	2	3	4	5	6
T_1	345.0	355.52	361.02	359.84	360.04	360.03	360.03
V_1	10.0	41.68	25.02	20.86	22.23	22.35	22.35
$S(t_f)$	15.0	62.46	42.47	44.63	44.53	44.53	44.53
J	-	148.72	90.06	100.24	99.47	99.44	99.44

Table 35. Convergence Rate of A(t), in problem 4E

ITER. / TIME	1	2	3	4	5	6
0.0	982.39	444.04	514.23	517.26	517.34	517.34
0.2	4.74	4.43	4.63	4.65	4.65	4.65
0.4	1.48	1.74	1.87	1.89	1.89	1.89
0.6	0.55	0.85	0.91	0.92	0.92	0.92
0.8	0.19	0.38	0.40	0.41	0.41	0.41
1.0	0.00	0.00	0.00	0.00	0.00	0.00

Table 36. Convergence Rates of T_1, V_1, $I(t_f)$, $S(t_f)$, and J, Problem 1F

ITER / TIME	0	1	2	3	4	5	6	7	8	9	10	11
T_1	345.00	310.68	435.71	378.45	369.64	369.19	349.08	360.18	357.83	360.15	360.40	360.40
V_1	15.00	-11.66	-11.61	11.33	-18.53	9.18	15.02	30.06	24.74	17.40	17.91	17.95
$I(t_f)$	10.00	-8.18	14.00	1.23	7.41	5.06	1.39	-1.72	-6.72	-6.54	-6.56	-6.56
$S(t_f)$	20.00	60.54	75.94	70.65	73.02	72.38	70.29	66.85	62.64	61.78	61.72	61.72
J	-	191.23	258.89	240.05	243.48	243.67	240.88	226.74	204.80	204.75	204.36	204.36

Table 37. Convergence Rate of A(t), Problem 1F

TIME \ ITER	1	2	3	4	5	6	7	8	9
0.0	1453.77	2019.26	2142.85	2305.12	2268.12	2092.78	1801.76	1517.04	1516.05
0.2	4.36	3.96	4.10	4.18	4.20	4.13	4.05	3.93	3.96
0.4	1.54	1.52	1.61	1.66	1.67	1.63	1.58	1.52	1.55
0.6	0.75	0.72	0.77	0.79	0.80	0.78	0.78	0.78	0.80
0.8	0.36	0.29	0.32	0.32	0.32	0.32	0.35	0.38	0.38
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 38. Convergence Rates of T_1, V_1, $I(t_f)$, $S(t_f)$, and J, problem 2G

ITER.	0	1	2	3	4	5
T_1	370.00	362.71	360.67	360.79	360.83	360.83
V_1	9.00	14.04	18.95	20.20	20.31	20.31
$I(t_f)$	4.00	3.56	4.03	4.06	4.06	4.06
$S(t_f)$	30.00	45.41	53.96	54.03	54.03	54.03
J	-	109.52	110.22	110.25	110.23	110.23

Table 39. Convergence Rate of A(0), problem 2G

ITER / TIME	1	2	3	4	5
0.0	492.12	638.38	638.33	638.49	638.50
0.2	3.97	4.85	4.85	4.85	4.85
0.4	1.97	2.13	2.13	2.13	2.13
0.6	1.16	1.15	1.15	1.15	1.15
0.8	0.61	0.55	0.55	0.55	0.55
1.0	0.00	0.00	0.00	0.00	0.00

Table 40. Convergence Rates of T_1, V_1, $I(t_f)$, $S(t_f)$, and J, problem 2H

ITER	0	1	2	3	4	5	6	7
T_1	345.0	346.22	358.39	361.74	360.95	360.61	360.60	360.60
V_1	15.0	60.83	17.41	27.41	18.38	18.97	19.00	19.00
$I(t_f)$	3.0	0.91	-5.27	-3.39	-3.39	-3.41	-3.41	-3.41
$S(t_f)$	20.0	46.44	59.06	59.18	58.98	58.93	58.93	58.93
J	-	115.96	147.58	147.79	148.86	148.50	148.50	148.50

Table 41. Convergence Rate of A(t), problem 2H

TIME \ ITER	1	2	3	4	5	6	7
0.0	1689.52	1077.35	1195.87	1186.12	1183.06	1182.98	1182.98
0.2	4.35	3.92	4.14	4.16	4.16	4.16	4.16
0.4	2.06	1.54	1.69	1.70	1.70	1.70	1.70
0.6	1.33	0.81	0.89	0.90	0.90	0.90	0.90
0.8	0.86	0.41	0.44	0.44	0.44	0.44	0.44
1.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00

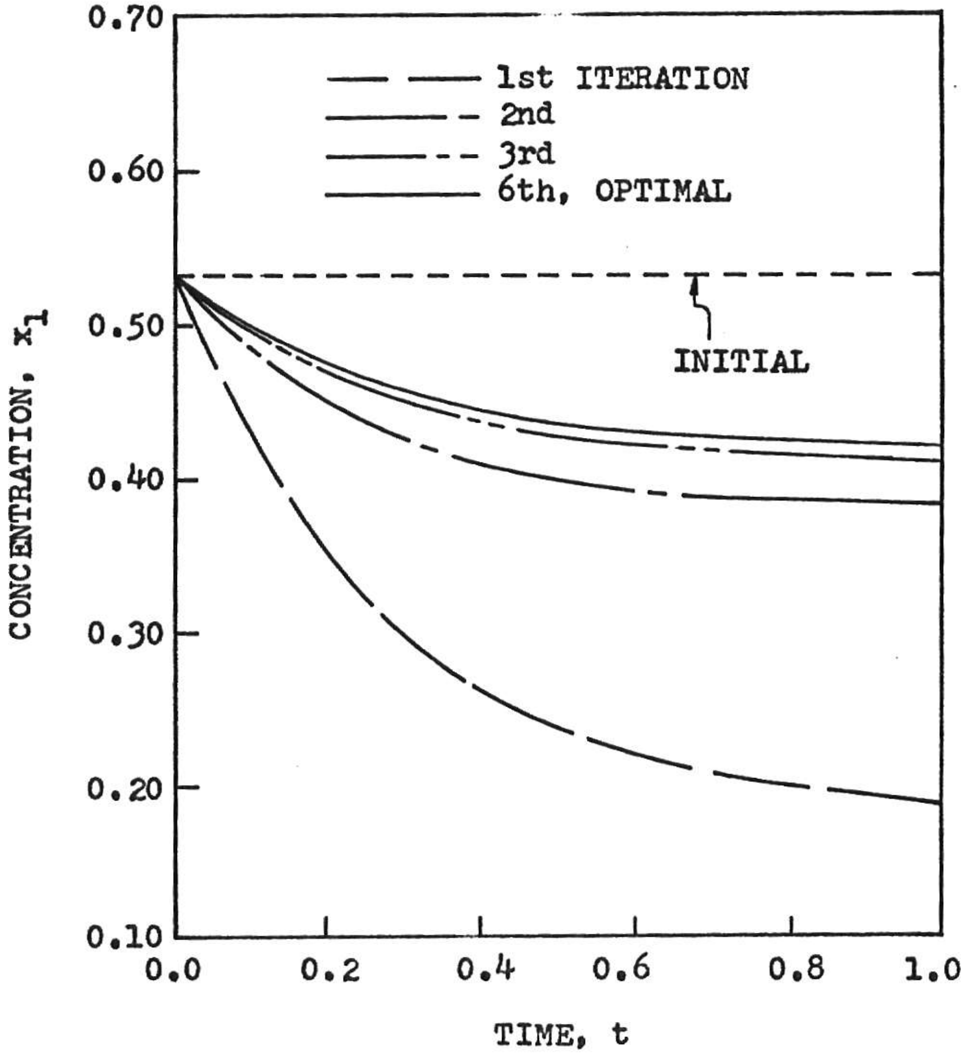

Fig. 28. Convergence Rate of Concentration x_1, Problem 5A

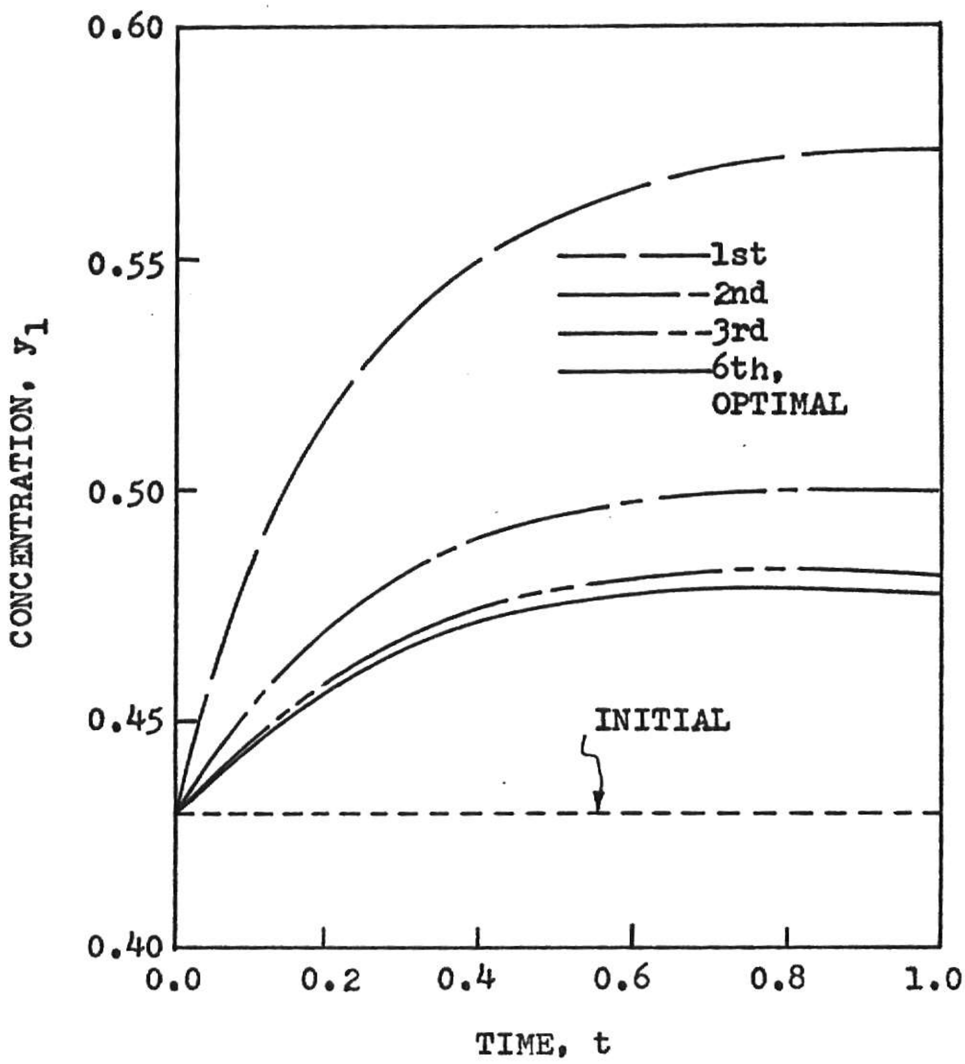

Fig. 29. Convergence Rate of Concentration y_1, Problem 5A

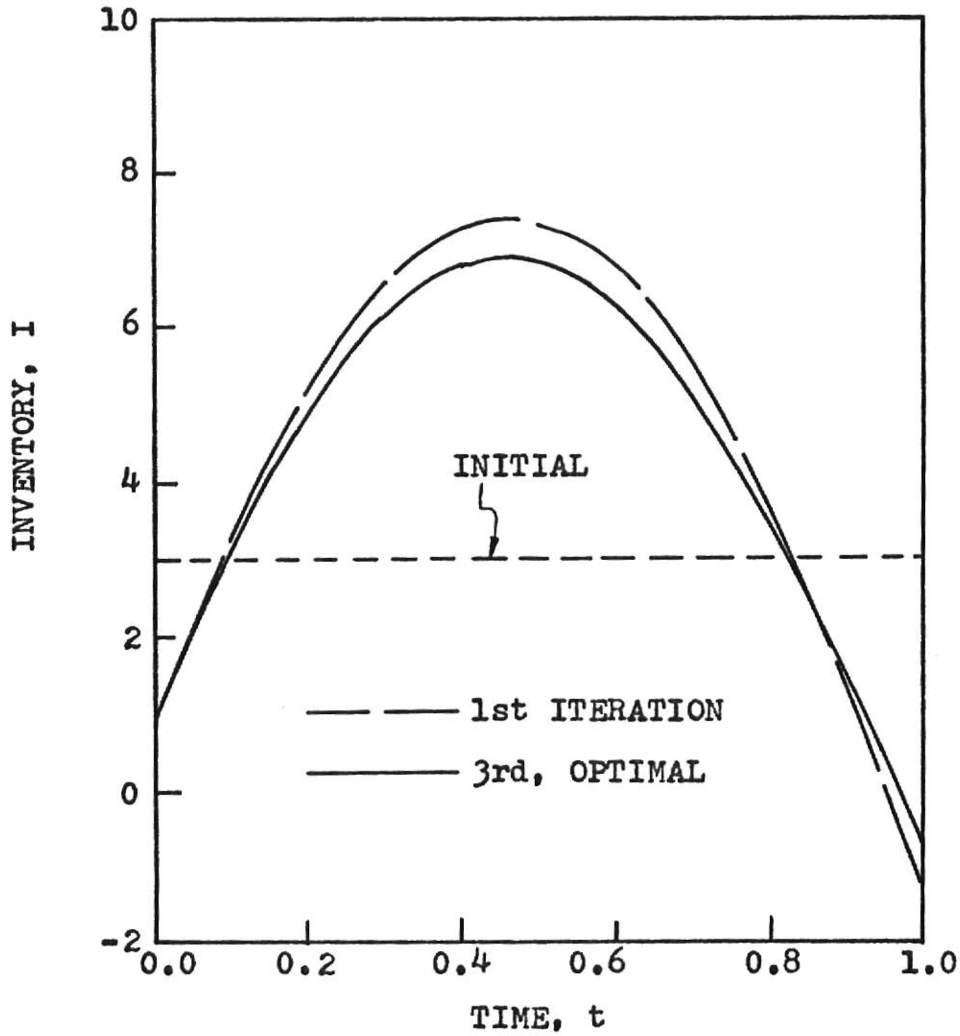

Fig. 30. Convergence Rate of Inventory I, Problem 5A

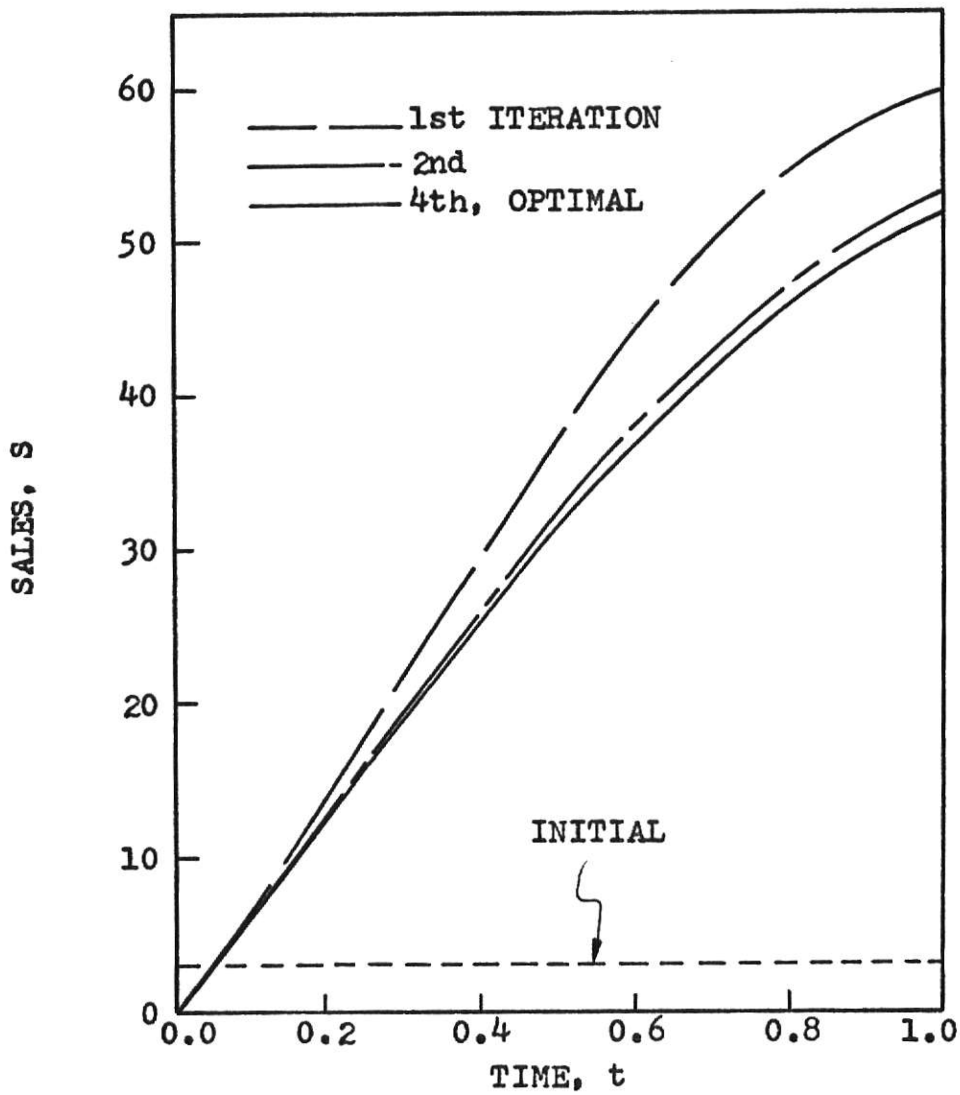

Fig. 31. Convergence Rate of Sales S, Problem 5A

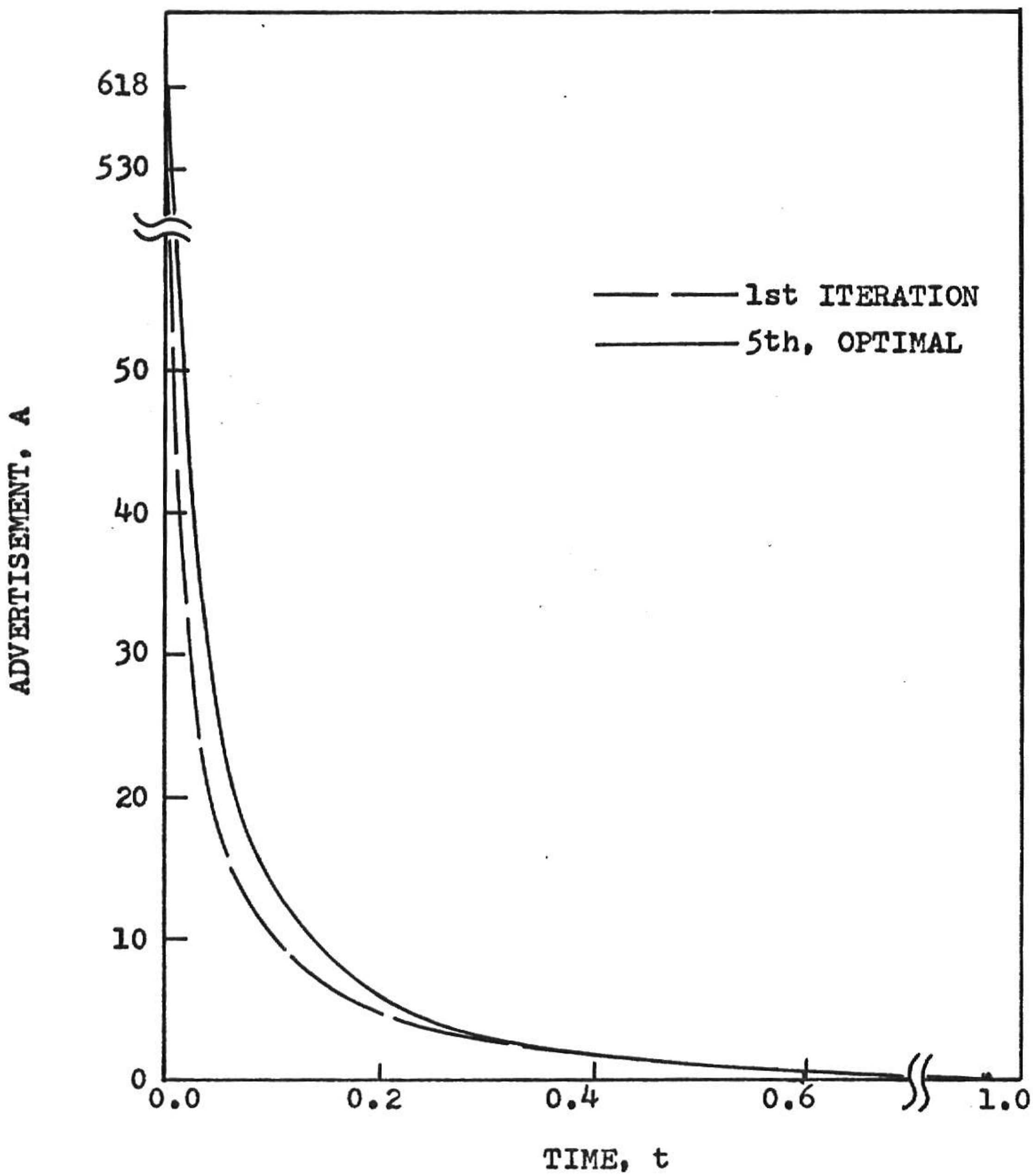

Fig. 32. Convergence Rate of A, Problem 5A

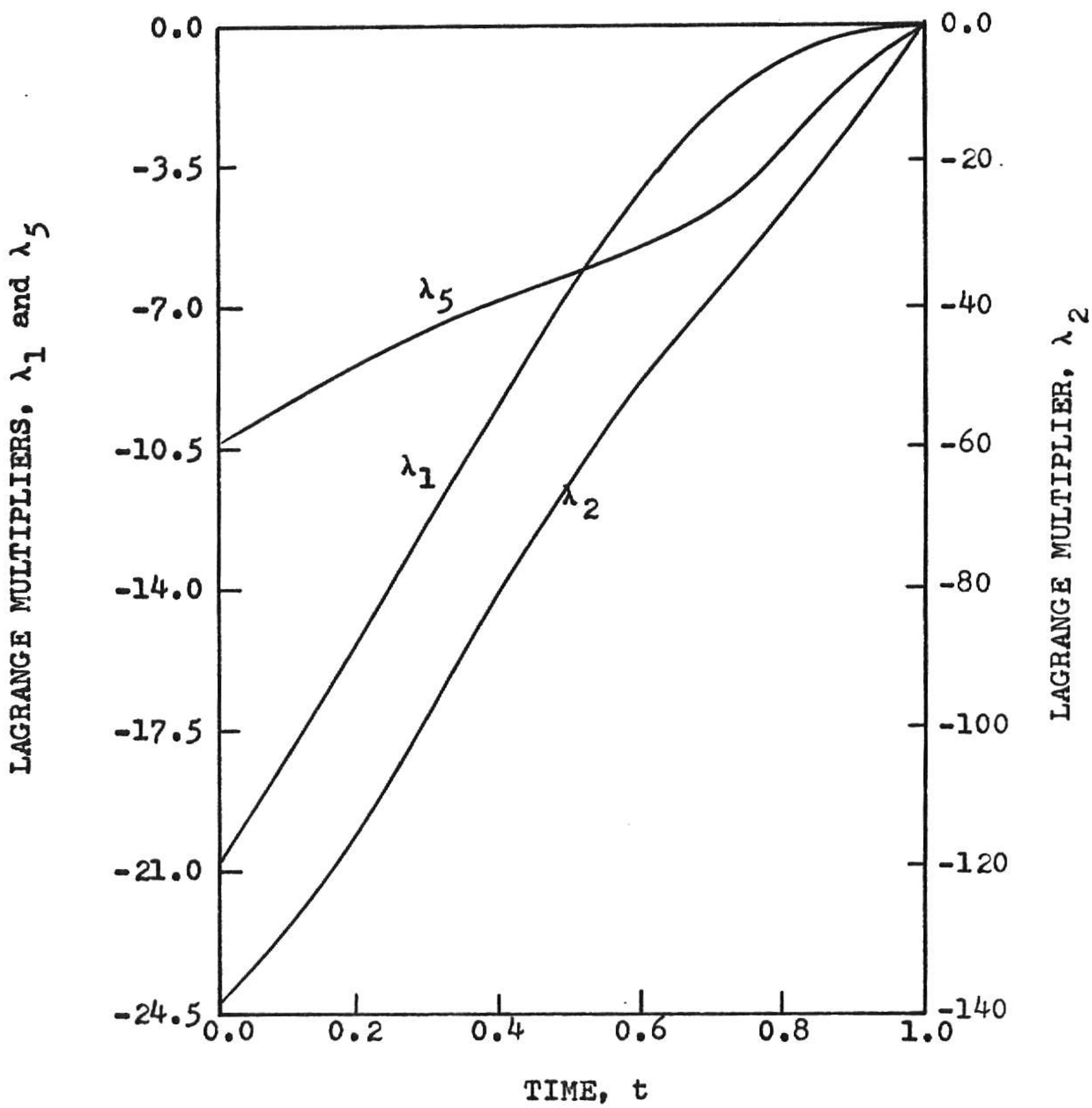

Fig. 33. Optimal Profiles of λ_1, λ_2 and λ_5, Problem A

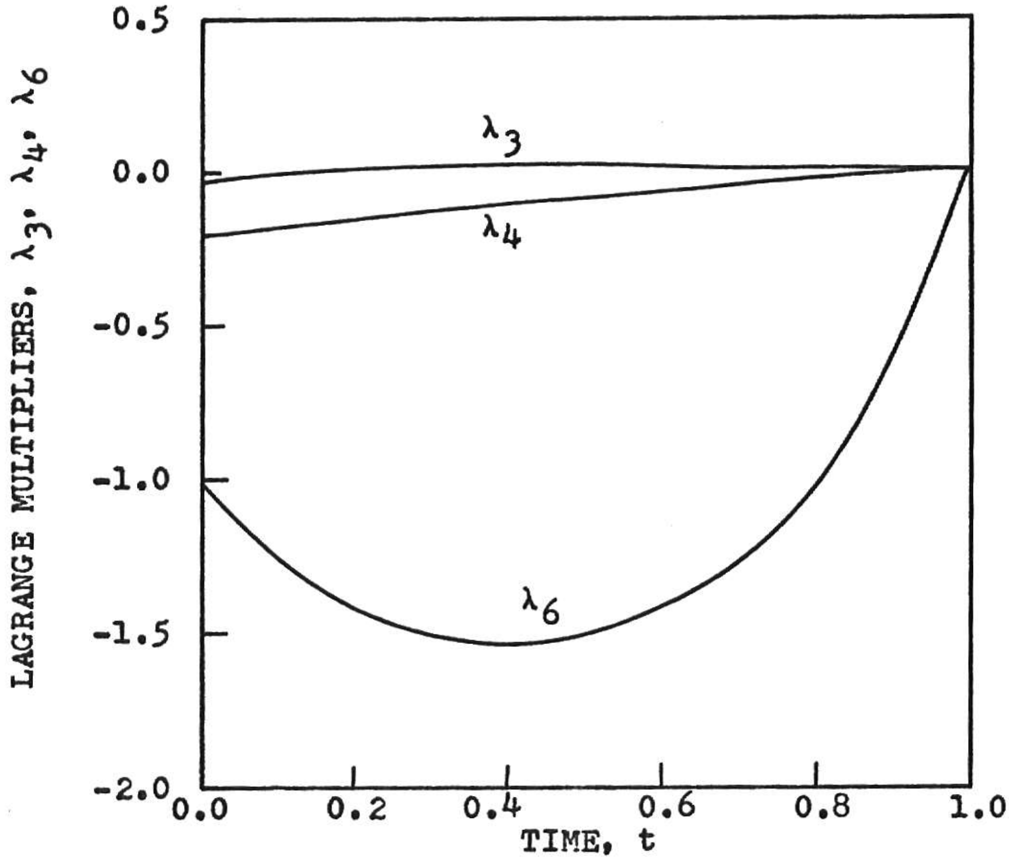

Fig. 34. Optimal Profiles of λ_3, λ_4 and λ_6, Problem A

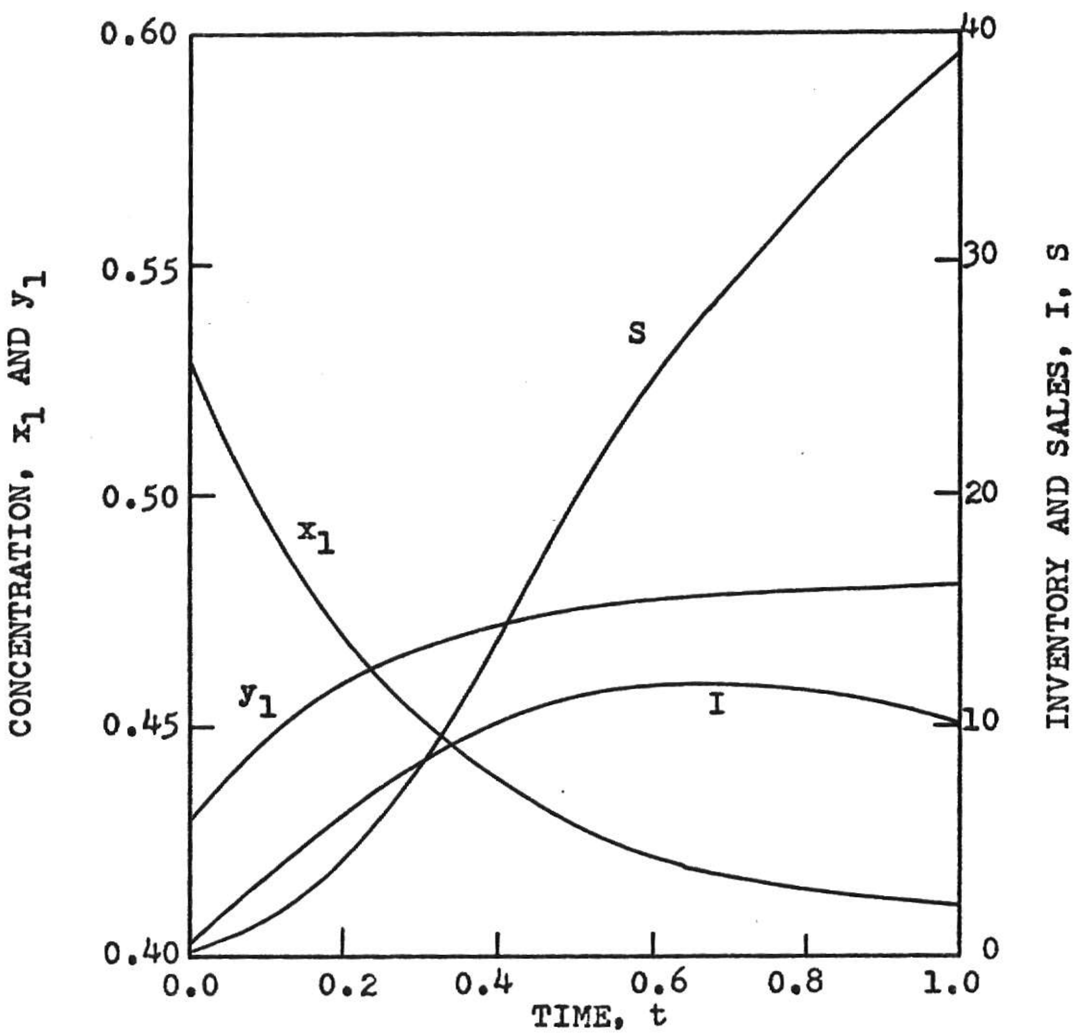

Fig. 35. Optimal Profiles of x_1, y_1, I, S, Problem D.

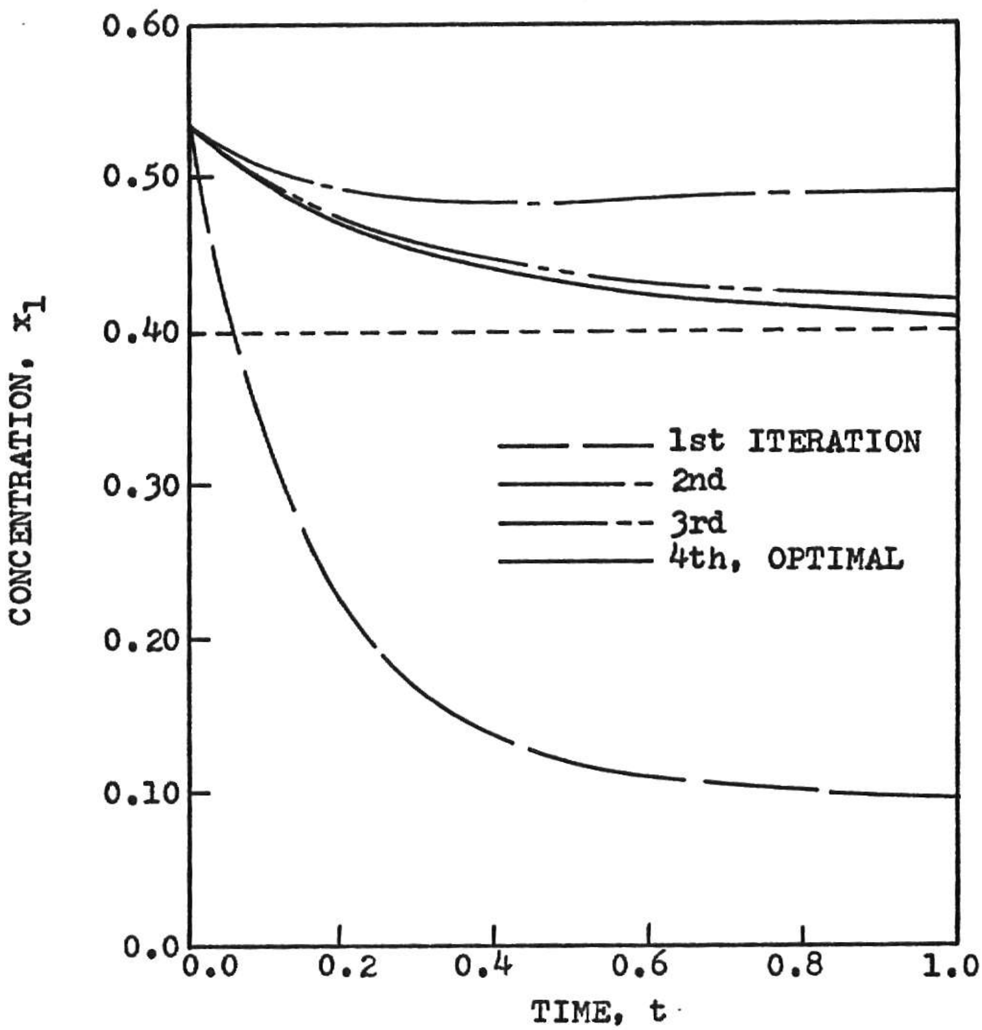

Fig. 36. Convergence Rate of Concentration x_1, Problem 4E

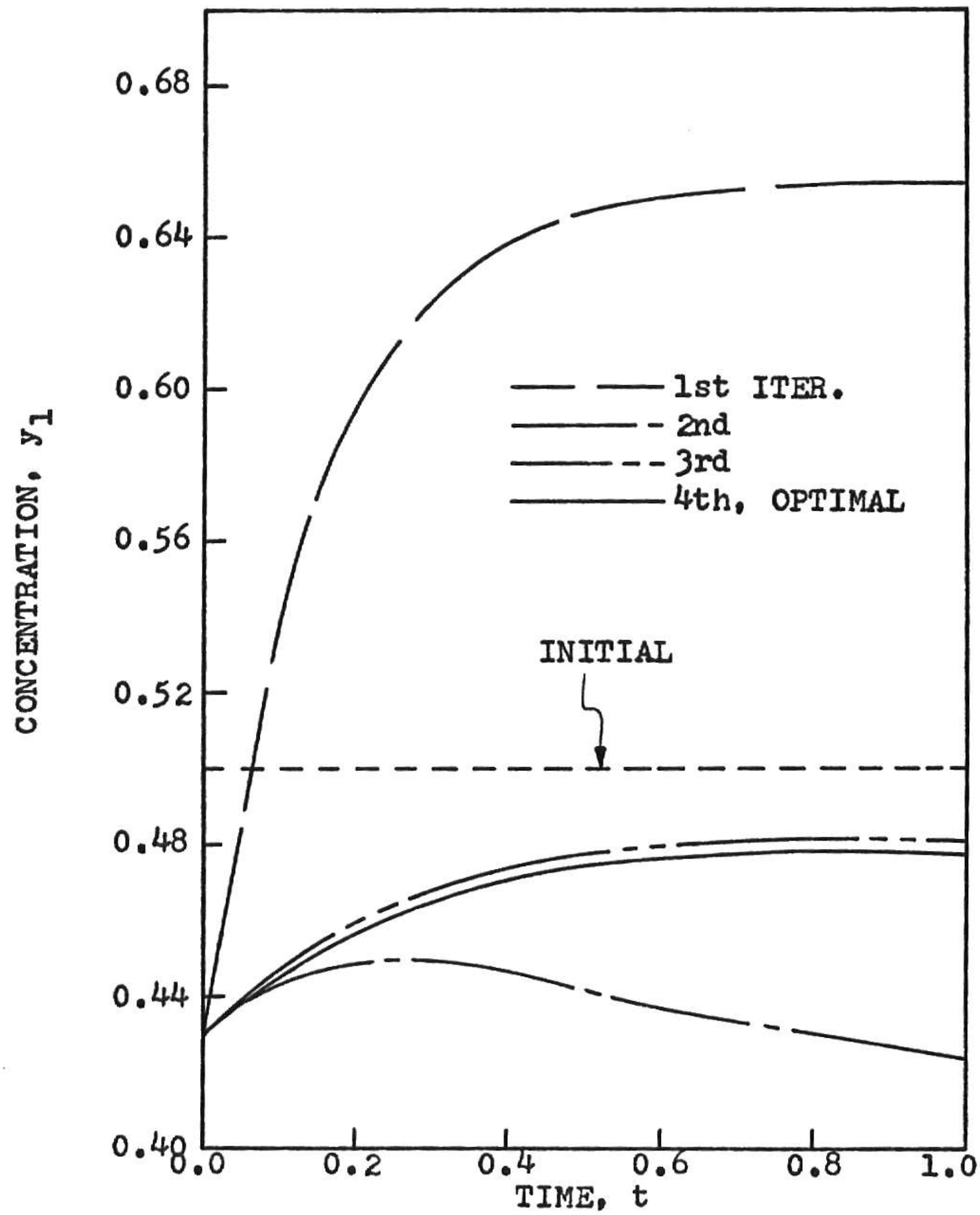

Fig. 37. Convergence Rate of Concentration y_1 Problem 4E

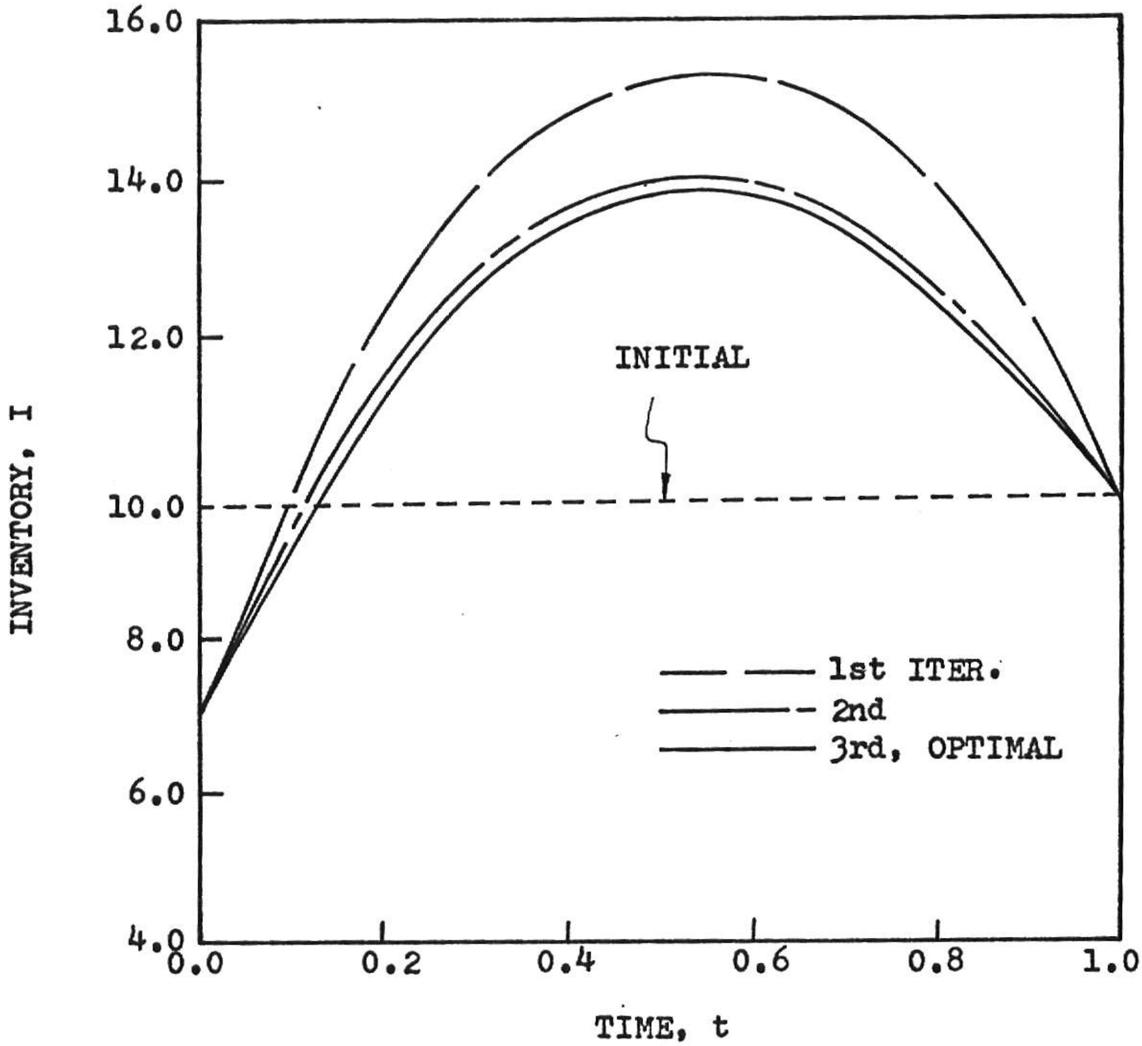

Fig. 38. Convergence Rate of I, Problem 4E

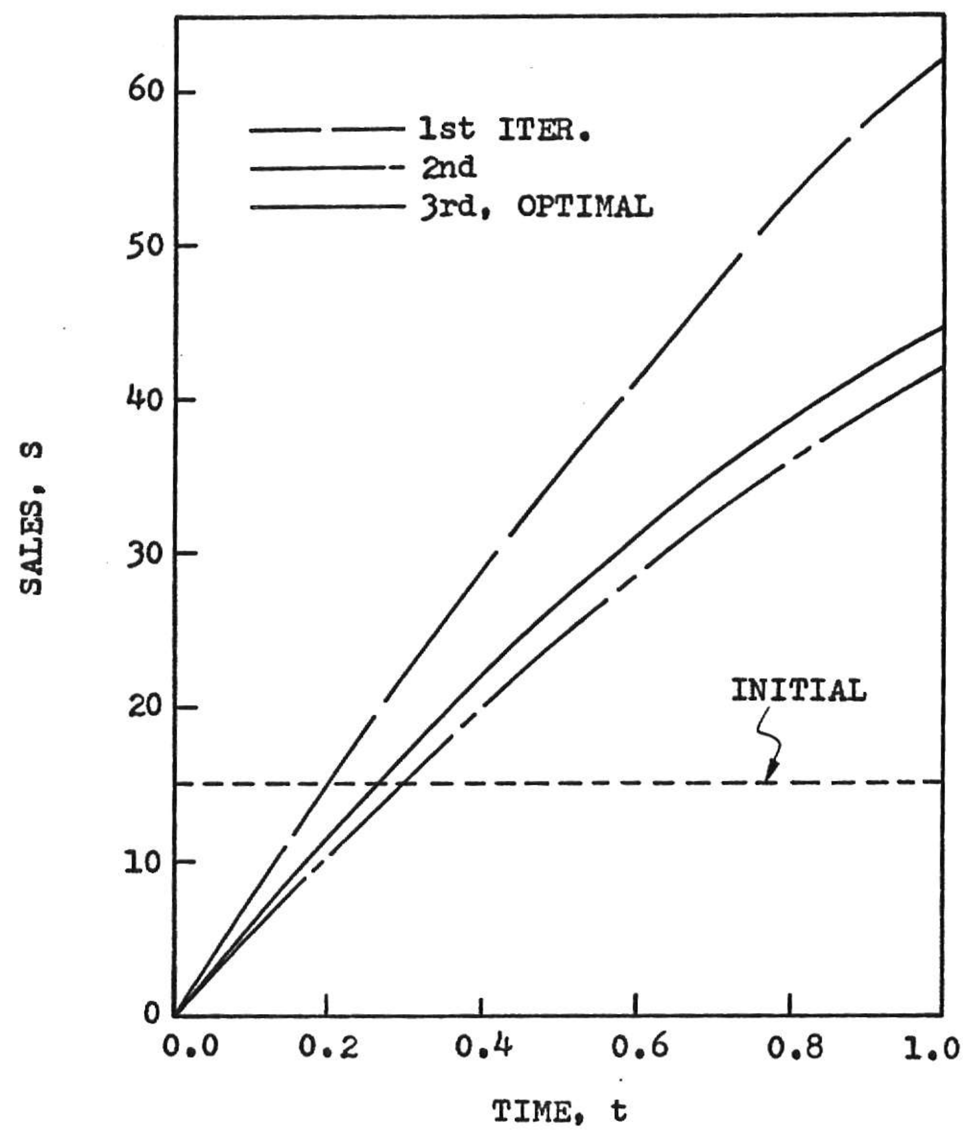

Fig. 39. Convergence Rate of S, Problem 4E

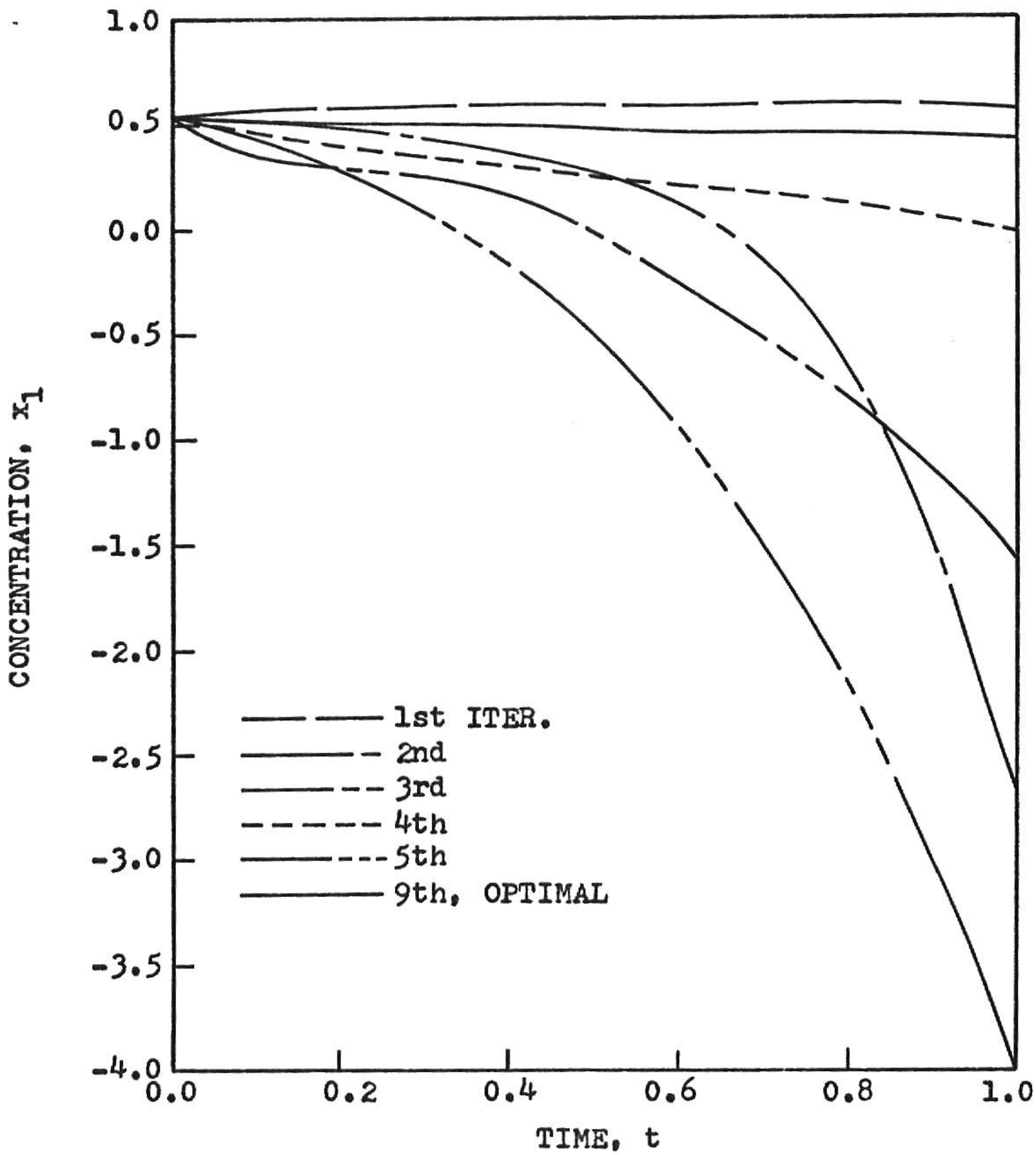

Fig. 40. Convergence Rate of Concentration x_1 Problem 1F

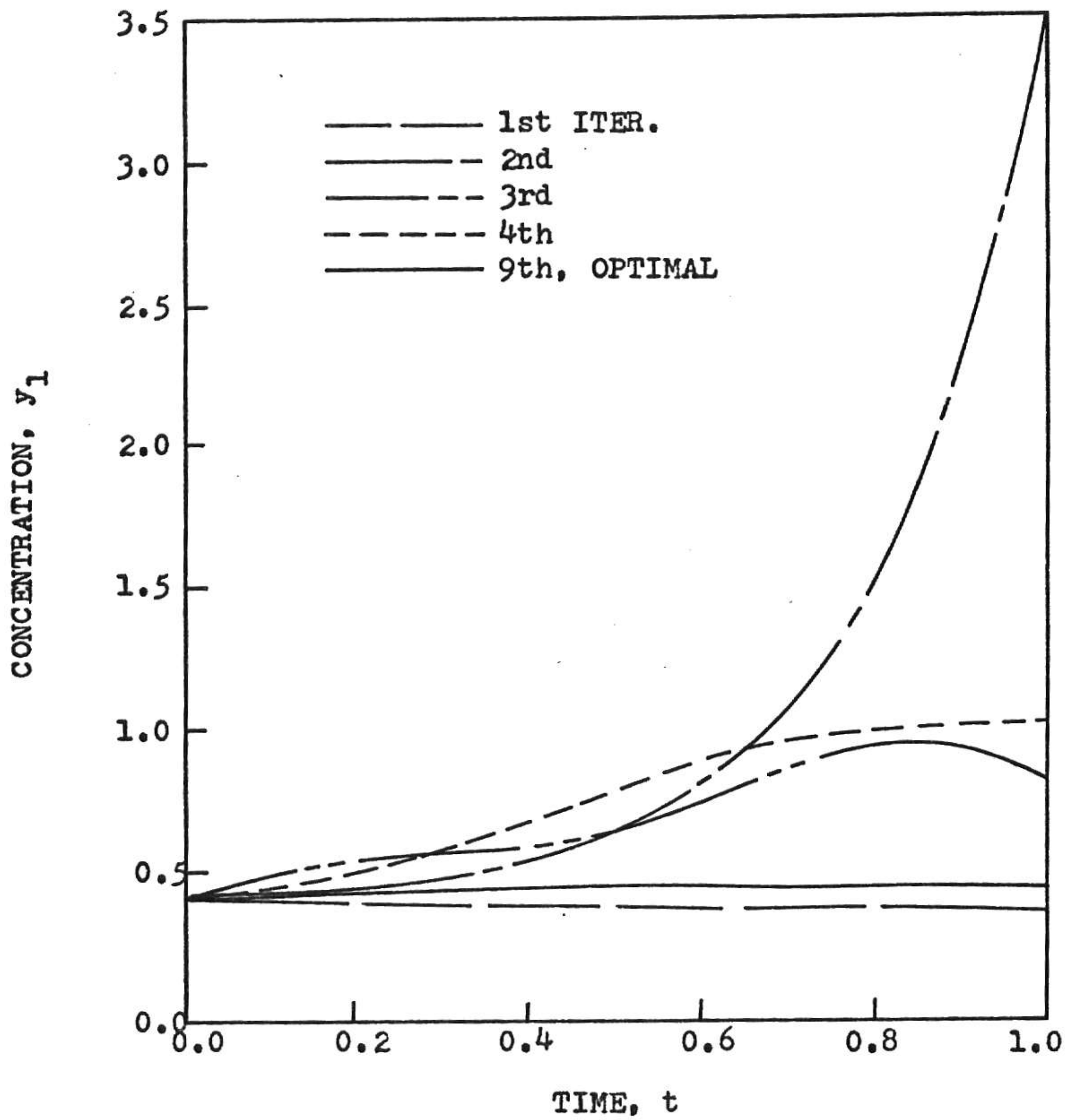

Fig. 41. Convergence Rate of Concentration y_1, Problem 1F

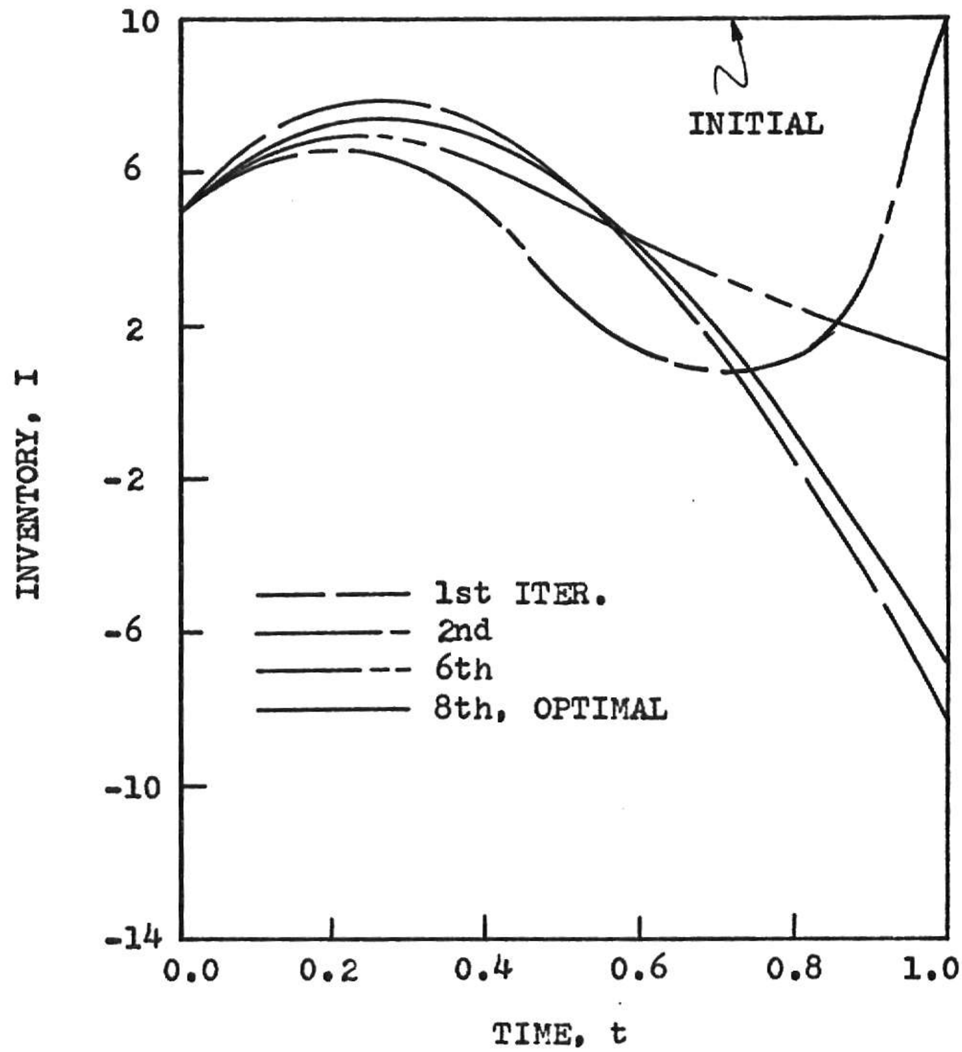

Fig. 42. Convergence Rate of I, Problem 1F

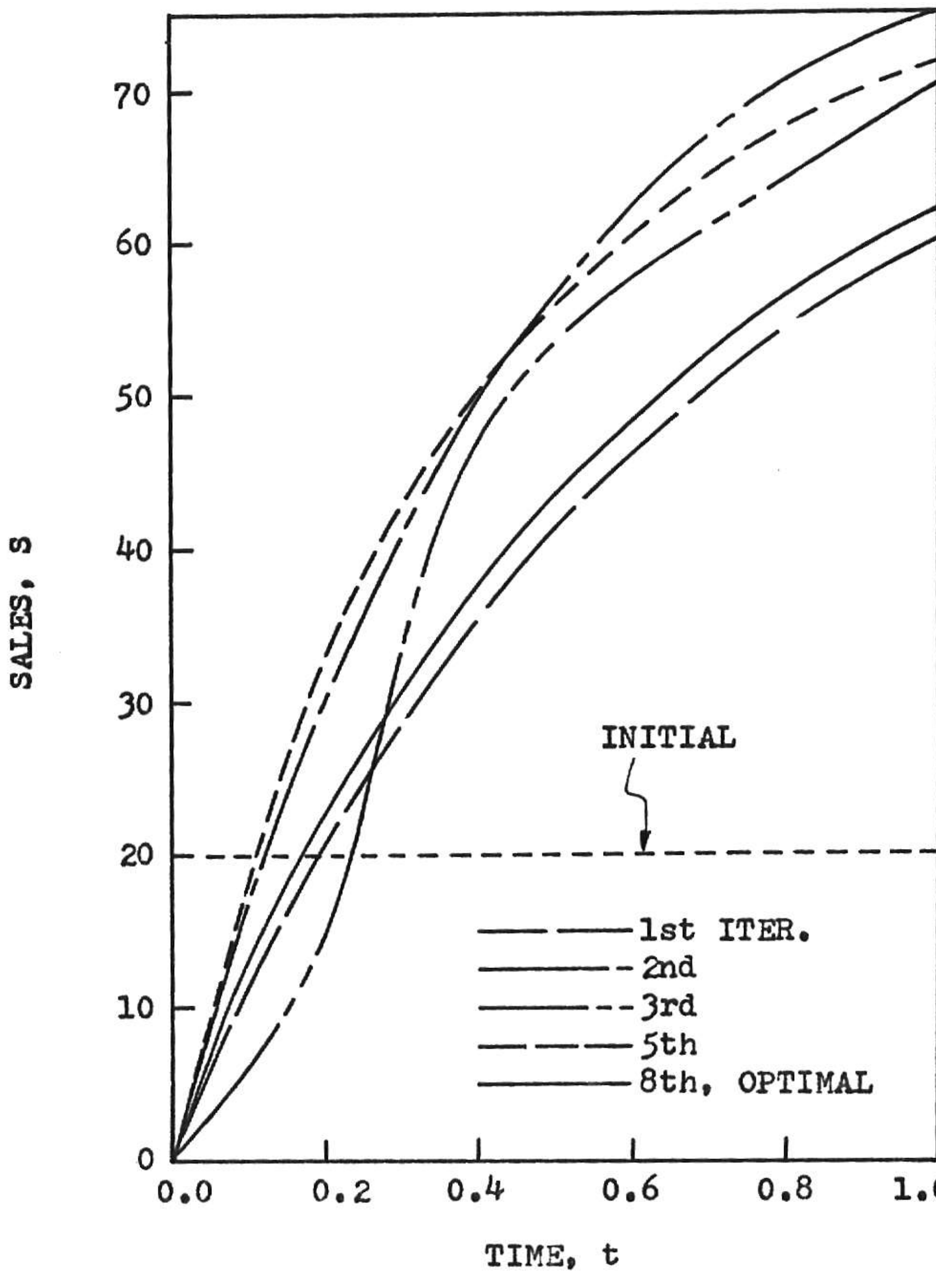

Fig. 43. Convergence Rate of S, Problem 1F

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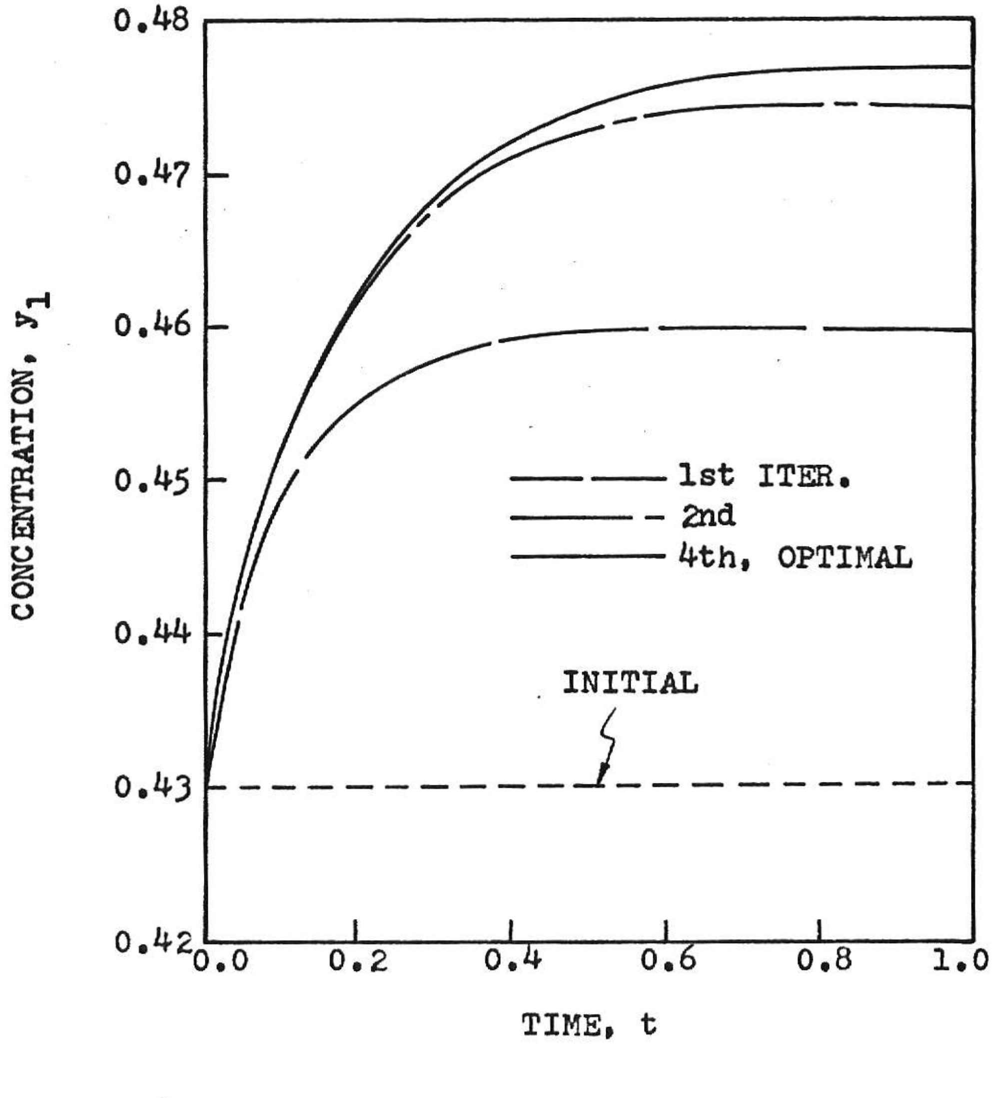

Fig. 45. Convergence Rate of Concentration y_1, Problem 2G

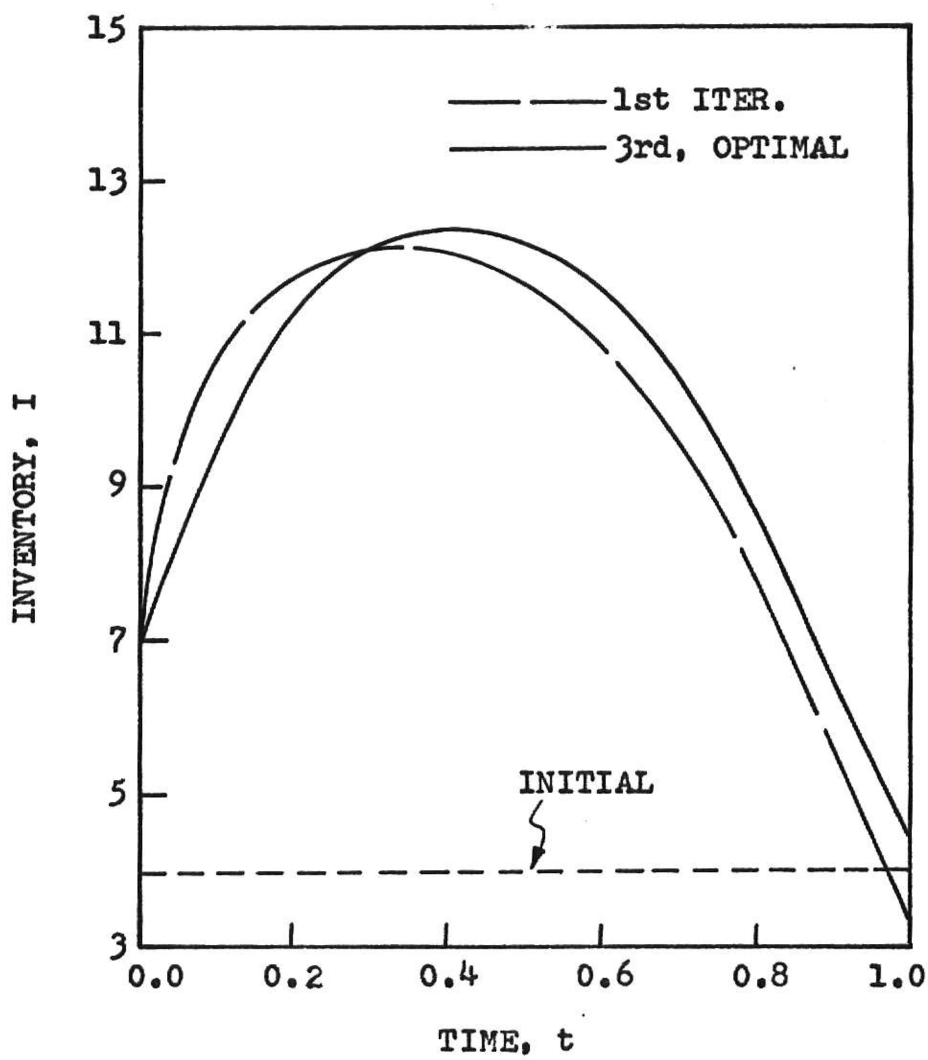

Fig. 46. Convergence Rate of I, Problem 2G

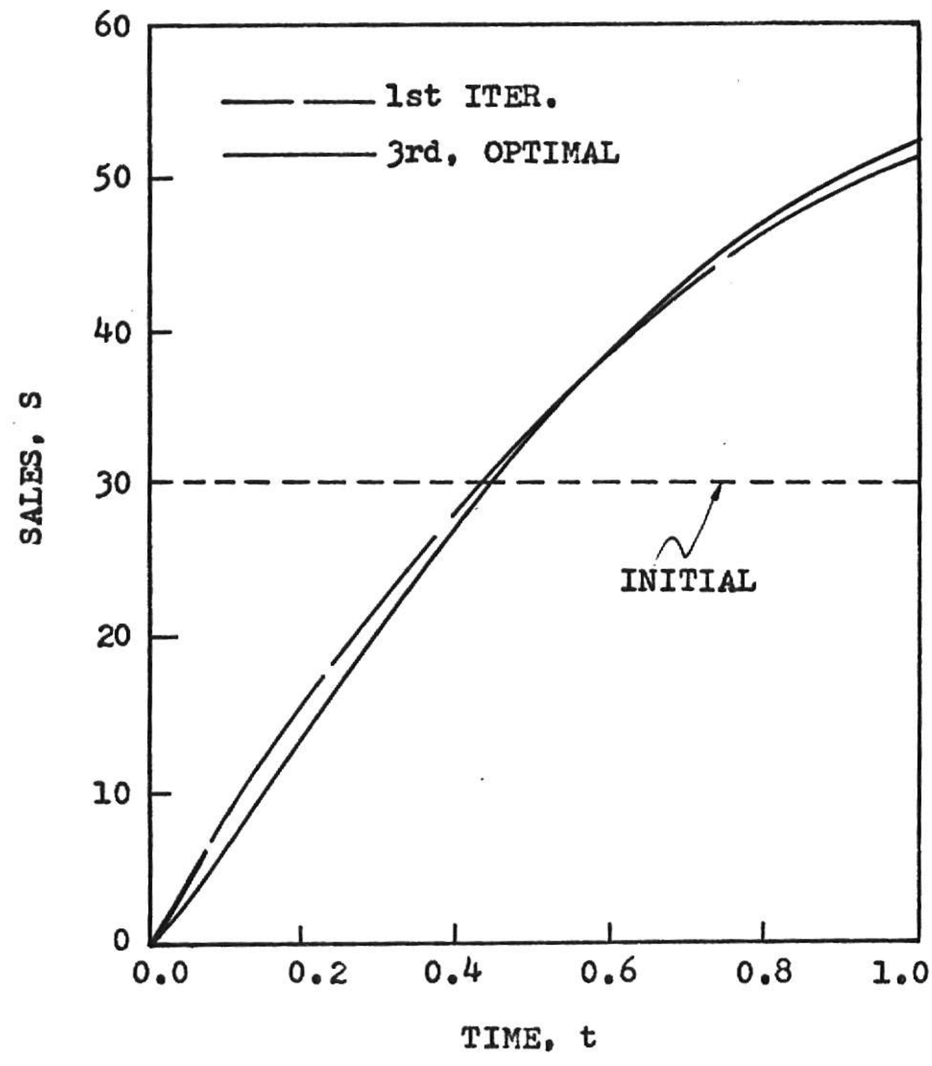

Fig. 47. Convergence Rate of S, Problem 2G

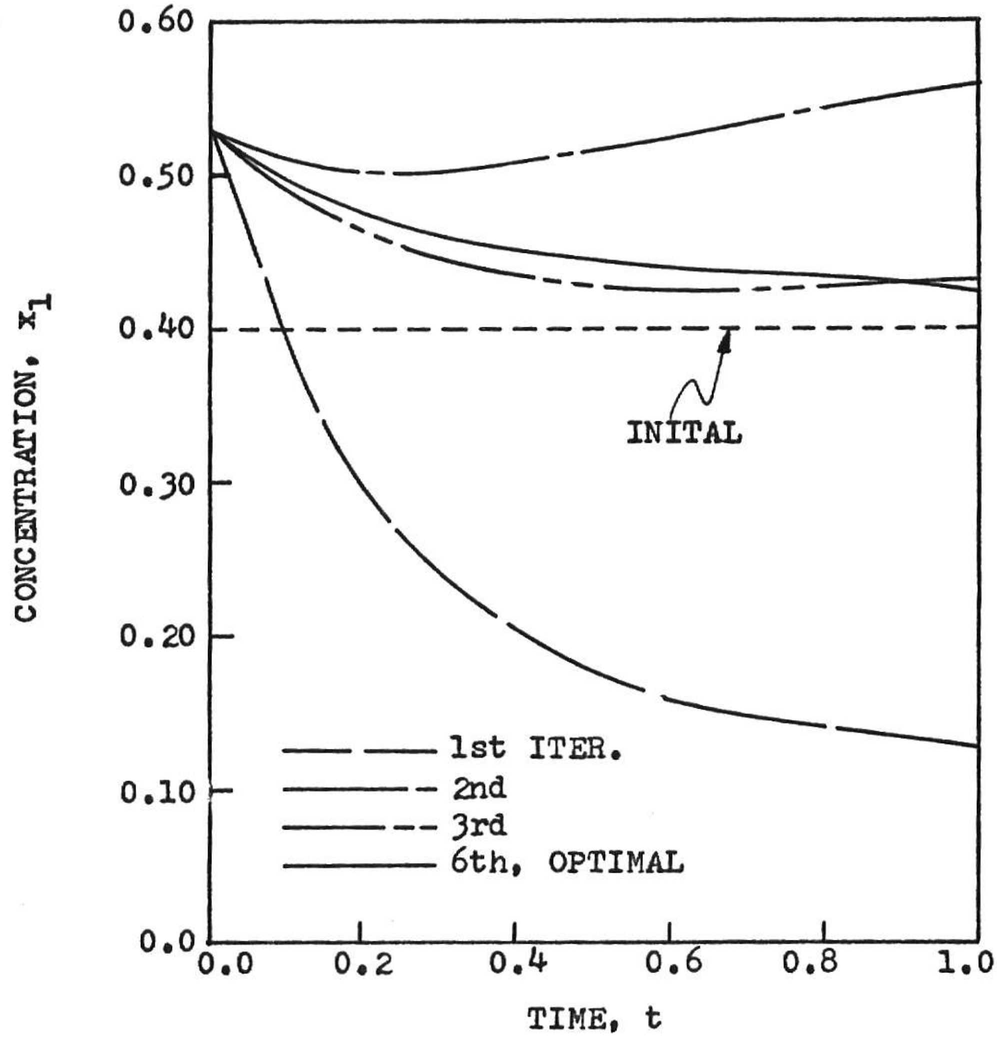

Fig. 48. Convergence Rate of Concentration x_1
Problem 2H

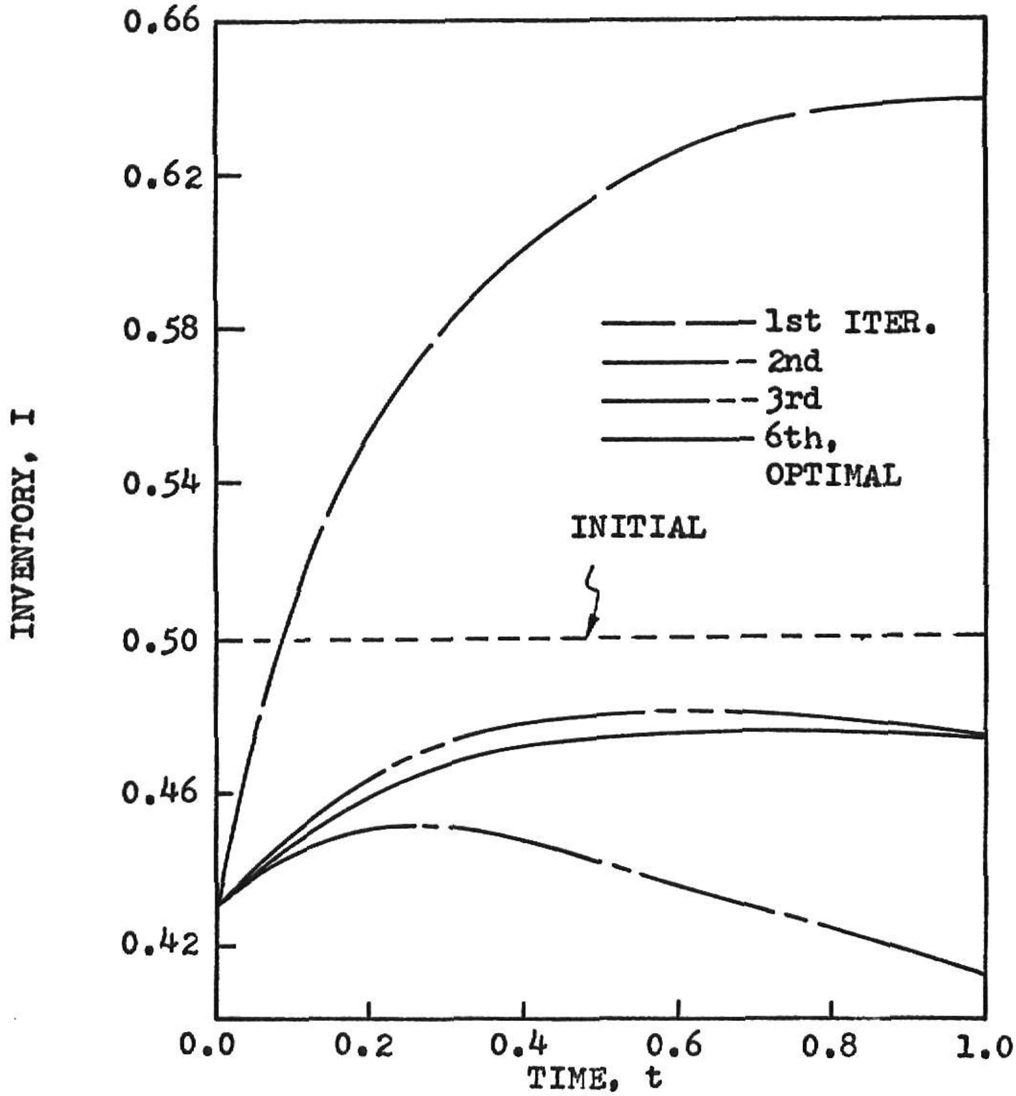

Fig. 49. Convergence Rate of Concentration y_1, Problem 2H

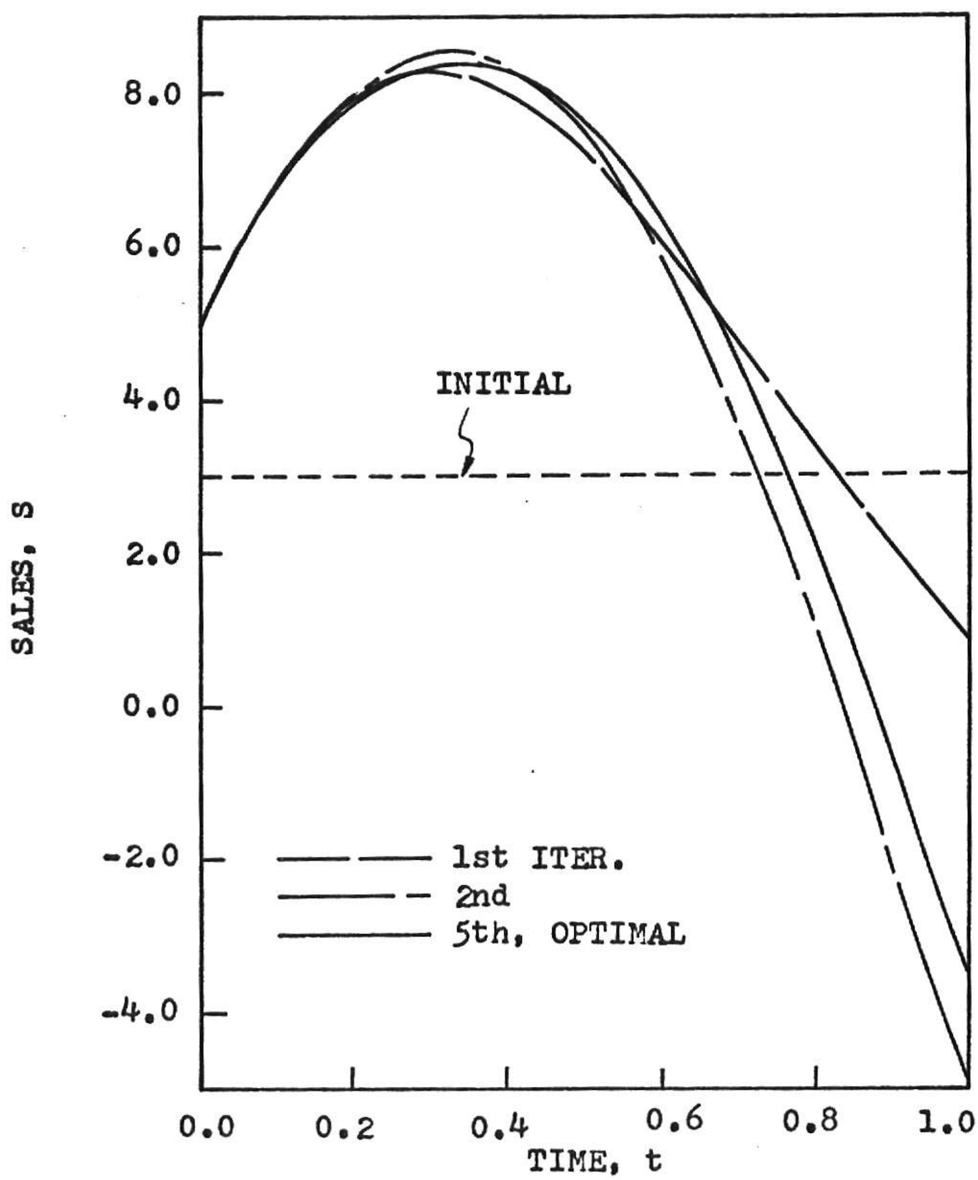

Fig. 50. Convergence Rate of I, Problem 2H

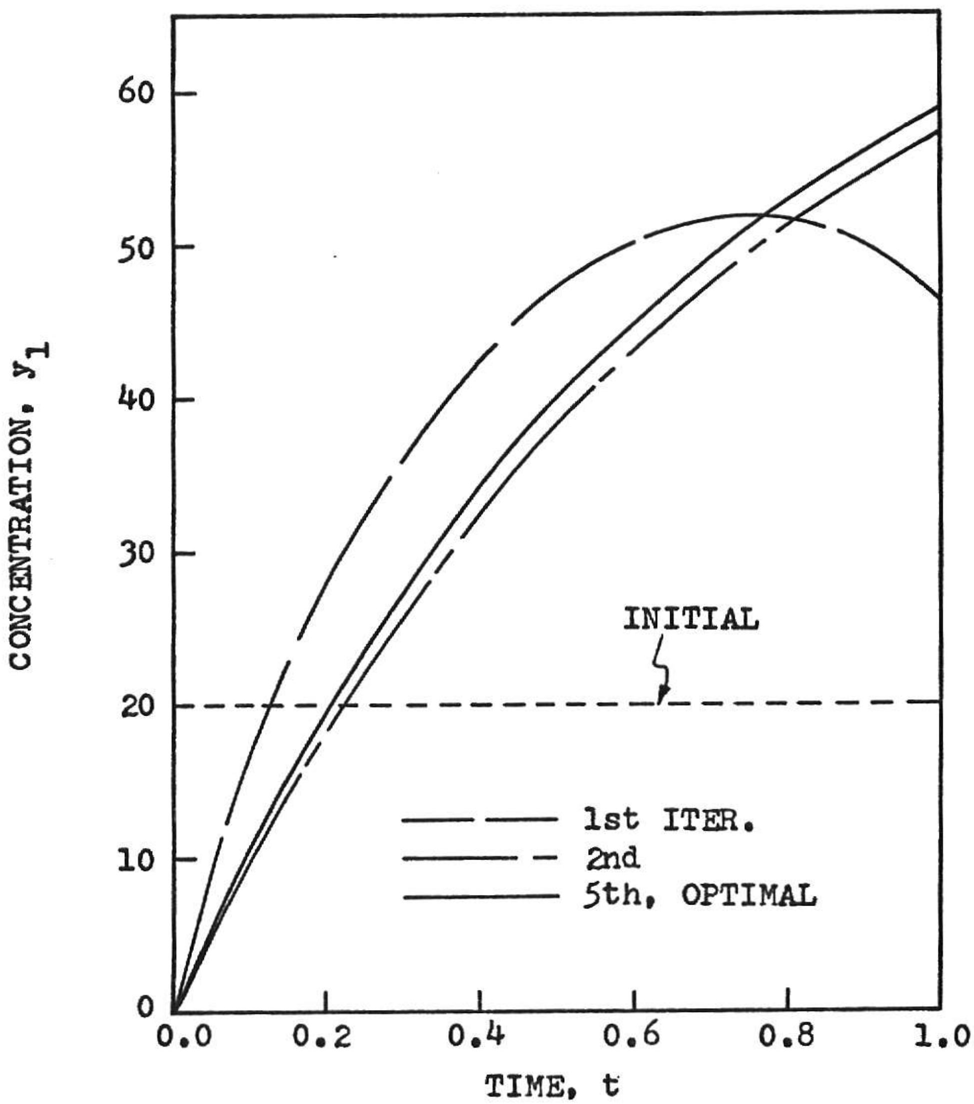

Fig. 51. Convergence Rate of S, Problem 2H

CHAPTER 6

CONCLUSION

The examples solved in this thesis show that quasilinearization is an effective tool for obtaining numerical solutions of industrial management problem. It also shows that this technique is equally effective for the simultaneous optimization of the control variables and the unknown parameters. The results show that the addition of unknown parameters in the problem does not significantly increase the amount of computation.

The convergence rate of the problem solved in Chapter 4 was found very rapid. Choosing the correct initial approximation was not difficult. Convergence was obtained with most of the initial guesses. Notice that some of the initial approximations used are very poor and would not be used with a little engineering judgement.

In Chapter 5, with the addition of the volume of the reactor as an unknown parameter, the problem becomes more unstable. Among all the 29 initial approximations used, only 13 of them converged to the true solution. Since the parameter space for this particular problem in which convergence will occur is rather narrow, convergence difficulty exists. This can be seen especially in problem B, C, and G.

The quasilinearization technique has a main disadvantage which is the small convergence interval. Convergence only occurs when the initial guess is near the true solution. The method of steepest decent, on the other hand, is known to work very well in regions far removed from the true solution but very poorly in areas near the solution. We can use the method of steepest descent at the begining and then switch to quasilinearization when better approximations are obtained. By the proper use of these two methods, the convergence region should be increased.

Recently, Mehrotra [18] has used the two phase method of quasilinearization to enlarge the convergence interval of a production planning problem. Other techniques such as perturbation [19] and gradient technique [20] can also be used to improve the convergence.

APPENDIX 1

COMPUTER PROGRAM USED IN CHAPTER 4

```
C
C
C     THIS PROGRAM SOLVES A SET OF 16 DIFF. EQUATIONS TWO-POINT
C     SPLIT TYPE USING THE SUPERPOSITION PRINCIPLE AND RUNGE-
C     KUTTA TECHNIQUE
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Z(16, 51),X(16),FF(16, 51),ZN(16, 51),J1(16,16),
     1 B(16),ZP(16, 51),ZH(10,16, 51),ZFC(16),RZ(16),RM(4,16),F(16)
     2 ,A(105),ADV(51)
      DOUBLE PRECISION J1
      COMMON ZN,J1,RM,RZ,B,DT,M,N
C
C     READ IN DATA
C
      READ(1,905) GA,GB,EA,EB,R,Q,V1,V2
      READ(1,900) AIM,AN,CC,CT,T1M,XO,YO,DT
      READ(1,900) CQ,C1,C2,C3,CI,CA
C
C     ECHO CHECK
C
      WRITE(3,945) GA,GB,EA,EB,R,Q,V1,V2
      WRITE(3,950) AIM,AN,CC,CT,T1M,XO,YO,DT
      WRITE(3,955) CQ,C1,C2,C3,CI,CA
C
C
      NO=0
      M=16
      IGD=1./DT+1
      EPS=0.0000001
C
C     INITIAL APPROXIMATION
C
      DO 10 J=1,IGD
      Z(1,J)=0.53
      Z(2,J)=0.43
      Z(3,J)=0.53
      Z(4,J)=0.43
      Z(5,J) =18.
      Z(6,J)=10.
      Z(7,J)=350.
      Z(8,J)=350.
      Z(9,J)=-5.
      Z(10,J)=-10.
      Z(11,J)=-5.
      Z(12,J)=-15.
      Z(13,J)=-5.
      Z(14,J)=-1.
      Z(15,J)=0.
```

```
      Z(16,J)=0.
   10 CONTINUE
   15 CONTINUE
      WRITE(3,910) (J,(Z(I,J),I=1,10),J=1,IGD,10)
      WRITE(3,911)(J,(Z(I,J),I=11,16),J=1,IGD,10)
      DO 50 J=1,IGD
      DO 20 I=1,M
   20 X(I)=Z(I,J)
      CALL FFUNC(GA,GB,EA,EB,R,Q,V1,V2,AIM,AN,CC,CQ,C1,C2,C3,CI,CA,
     1 XO,YO, X,F)
      DO 30 I=1,M
   30 FF(I,J)=F(I)
   50 CONTINUE
C
C     PARTICULAR SOLUTION
C
      MH=0
      ZN(1,1)=0.53
      ZN(2,1)=0.43
      ZN(3,1)=0.53
      ZN(4,1)=0.43
      ZN(5,1)=12.
      ZN(6,1)=0.1
      DO 60 I=7,M
   60 ZN(I,1)=0.0
  500 CONTINUE
      DO 200 N=1,IGD
      AT1=DEXP(-EA/(R*Z(7,N)))*GA
      BT1=DEXP(-EB/(R*Z(7,N)))*GB
      AT2=DEXP(-EA/(R*Z(8,N)))*GA
      BT2=DEXP(-EB/(R*Z(8,N)))*GB
      AT11=EA/(R*Z(7,N)*Z(7,N))
      BT11=EB/(R*Z(7,N)*Z(7,N))
      AT22=EA/(R*Z(8,N)*Z(8,N))
      BT22=EB/(R*Z(8,N)*Z(8,N))
      J1(1,1)=-Q/V1-AT1
      J1(1,7)=-Z(1,N)*AT1*AT11
      J1(2,2)=-Q/V1-BT1
      J1(2,1)=AT1
      J1(2,7)=Z(1,N)*AT1*AT11-Z(2,N)*BT1*BT11
      J1(3,1)=Q/V2
      J1(3,3)=-Q/V2-AT2
      J1(3,8)=-Z(3,N)*AT2*AT22
      J1(4,2)=Q/V2
      J1(4,3)=AT2
      J1(4,4)=-Q/V2-BT2
      J1(4,8)=Z(3,N)*AT2*AT22-Z(4,N)*BT2*BT22
      J1(5,4)=C
      J1(5,6)=-1.
      J1(6,6)=CC+Z(14,N)/(CA*AN)-2.*CC *Z(6,N)/AN-Z(6,N)*Z(14,N)/
```

```
1 (CA*AN*AN)
 J1(6,14)=Z(6,N)/(CA*AN)-0.5/CA-0.5*Z(6,N)*Z(6,N)/(CA*AN*AN)
 J1(9,7)=(Z(9,N)-Z(10,N))*AT1*AT11
 J1(9,9)=Q/V1+AT1
 J1(9,10)=-AT1
 J1(9,11)=-Q/V2
 J1(10,7)=Z(10,N)*BT1*BT11
 J1(10,10)=Q/V1+BT1
 J1(10,12)=-Q/V2
 J1(11,8)=(Z(11,N)-Z(12,N))*AT2*AT22
 J1(11,11)=Q/V2+AT2
 J1(11,12)=-AT2
 J1(12,8)=Z(12,N)*BT2*BT22
 J1(12,12)=Q/V2+BT2
 J1(12,13)=-Q
 J1(13,5)=-2.*CI
 J1(14,6)=2.*CC*Z(14,N)/AN+Z(14,N)*Z(14,N)*0.5/(CA*AN*AN)
 J1(14,13)=1.
 J1(14,14)=-CC-Z(14,N)/(CA*AN)+2.*CC*Z(6,N)/AN+Z(6,N)*Z(14,N)
1 /(CA*AN*AN)
 J1(15,1)=(Z(9,N)-Z(10,N))*AT1*AT11
 J1(15,2)=Z(10,N)*BT1*BT11
 J1(15,7)=(Z(9,N)-Z(10,N))*AT1*AT11*(AT11-2./Z(7,N))*Z(1,N)+
1 Z(10,N)*BT1*Z(2,N)*BT11*(BT11-2./Z(7,N))
 J1(15,9)=Z(1,N)*AT1*AT11
 J1(15,10)=-Z(1,N)*AT1*AT11+Z(2,N)*BT1*BT11
 J1(16,3)=(Z(11,N)-Z(12,N))*AT2*AT22
 J1(16,4)=Z(12,N)*BT2*BT22
 J1(16,8)=(Z(11,N)-Z(12,N))*Z(3,N)*AT22*AT2*(AT22-2./Z(8,N))+
1 Z(12,N)*Z(4,N)*BT2*BT22*(BT22-2./Z(8,N))
 J1(16,11)=Z(3,N)*AT2*AT22
 J1(16,12)=-Z(3,N)*AT2*AT22+Z(4,N)*BT2*BT22
 IF(MH.NE.0) GO TO 110
 B(1)=-(J1(1,1)*Z(1,N)+J1(1,7)*Z(7,N))+FF(1,N)
 B(2)=-(J1(2,2)*Z(2,N)+J1(2,1)*Z(1,N)+J1(2,7)*Z(7,N))+FF(2,N)
 B(3)=-(J1(3,1)*Z(1,N)+J1(3,3)*Z(3,N)+J1(3,8)*Z(8,N))+FF(3,N)
 B(4)=-(J1(4,2)*Z(2,N)+J1(4,3)*Z(3,N)+J1(4,4)*Z(4,N)+J1(4,8)*
1 Z(8,N))+FF(4,N)
 B(5)=-(J1(5,4)*Z(4,N)+J1(5,6)*Z(6,N))+FF(5,N)
 B(6)=-(J1(6,6)*Z(6,N)+J1(6,14)*Z(14,N))+FF(6,N)
 B(7)=0.0
 B(8)=0.0
 B(9)=-(J1(9,7)*Z(7,N)+J1(9,9)*Z(9,N)+J1(9,10)*Z(10,N)+
1 J1(9,11)*Z(11,N))+FF(9,N)
 B(10)=-(J1(10,7)*Z(7,N)+J1(10,10)*Z(10,N)+J1(10,12)*Z(12,N))+
1 FF(10,N)
 B(11)=-(J1(11,8)*Z(8,N)+J1(11,11)*Z(11,N)+J1(11,12)*Z(12,N))+
1 FF(11,N)
 B(12)=-(J1(12,8)*Z(8,N)+J1(12,12)*Z(12,N)+J1(12,13)*Z(13,N))+
1 FF(12,N)
```

```
      B(13)=-(J1(13,5)*Z(5,N))+FF(13,N)
      B(14)=-(J1(14,6)*Z(6,N)+J1(14,13)*Z(13,N)+J1(14,14)*Z(14,N))+
     1 FF(14,N)
      B(15)=-(J1(15,1)*Z(1,N)+J1(15,2)*Z(2,N)+J1(15,7)*Z(7,N)+J1(15,9)
     1 *Z(9,N)+J1(15,10)*Z(10,N))+FF(15,N)
      B(16)=-(J1(16,3)*Z(3,N)+J1(16,4)*Z(4,N)+J1(16,8)*Z(8,N)+J1(16,11)
     1 *Z(11,N)+J1(16,12)*Z(12,N))+FF(16,N)
      GO TO 120
  110 DO 115 I=1,M
  115 B(I)=0.0
  120 CONTINUE
      CALL RUNGK
  200 CONTINUE
      IF(MH.NE.0) GO TO 300
      DO 220 J=1,IGD
      DO 220 I=1,M
      ZP(I,J)=ZN(I,J)
  220 CONTINUE
C
C     HOMOGENEOUS  SOLUTION
C
      MH=1
      DO 230 I=1,M
  230 ZN(I,1)=0.0
      ZN(7,1)=1.
      GO TO 500
  300 CONTINUE
      DO 350 J=1,IGD
      DO 350 I=1,M
  350 ZH(MH,I,J)=ZN(I,J)
      GO TO (420,430,440,450,460,470,480,490,501,510),MH
  420 MH=2
      DO 425 I=1,M
  425 ZN(I,1)=0.0
      ZN(8,1)=1.
      GO TO 500
  430 MH=3
      DO 435 I=1,M
  435 ZN(I,1)=0.0
      ZN(9,1)=1.
      GO TO 500
  440 MH=4
      DO 445 I=1,M
  445 ZN(I,1)=0.0
      ZN(10,1)=1.
      GO TO 500
  450 MH=5
      DO 455 I=1,M
  455 ZN(I,1)=0.0
      ZN(11,1)=1.
```

```
      GO TO 500
  460 MH=6
      DO 465 I=1,M
  465 ZN(I,1)=0.0
      ZN(12,1)=1.
      GO TO 500
  470 MH=7
      DO 475 I=1,M
  475 ZN(I,1)=0.0
      ZN(13,1)=1.
      GO TO 500
  480 MH=8
      DO 485 I=1,M
  485 ZN(I,1)=0.0
      ZN(14,1)=1.
      GO TO 500
  490 MH=9
      DO 495 I=1,M
  495 ZN(I,1)=0.0
      ZN(15,1)=1.
      GO TO 500
  501 MH=10
      DO 505 I=1,M
  505 ZN(I,1)=0.0
      ZN(16,1)=1.
      GO TO 500
  510 CONTINUE
C
C     BOUNDARY CONDITION
C
      DO 520 I=9,M
  520 ZFC(I)=0.0
      DO 550 J=1,10
      DO 530 I=9,16
      II=I-8
  530 J1(II,J)=ZH(J,I,IGD)
      J1(9,J)=2.*CT*(ZH(J,8,1)-2.*ZH(J,7,1))-ZH(J,15,1)
  550 J1(10,J)=2.*CT* (ZH(J,7,1)-ZH(J,8,1))-ZH(J,16,1)
      DO 570 I=9,16
      II=I-8
  570 B(II)=ZFC(I)-ZP(I,IGD)
      B(9)=ZP(15,1)-2.*CT*(ZP(8,1)-2.*ZP(7,1)+T1M)
      B(10)=ZP(16,1)-2.*CT*(ZP(7,1)-ZP(8,1))
      DO 580 J=1,10
      DO 580 I=1,10
      II=(J-1)*10+I
  580 A(II)=J1(I,J)
      CALL DGELG(B,A,10,1,EPS,IER)
C
C     GENERAL SOLUTION
```

```
C
      DO 620 J=1,IGD
      DO 620 I=1,M
      S=0.0
      DO 610 L=1,10
  610 S=S+B(L)*ZH(L,I,J)
  620 ZN(I,J)=ZP(I,J)+S
C
C     PRINT OUT SOLUTIONS
C
      NO=NO+1
      WRITE(3,912) NO
      WRITE(3,915)(J,(ZP(I,J),I=1,10),J=1,IGD,10)
      WRITE(3,911) (J,(ZP(I,J),I=11,16),J=1,IGD,10)
      DO 630 L=1,10
      WRITE(3,920) L,(J,(ZH(L,I,J),I=1,10),J=1,IGD,10)
  630 WRITE(3,911) (J,(ZH(L,I,J),I=11,16),J=1,IGD,10)
      WRITE(3,925) (B(I),I=1,10)
      WRITE(3,930) (J,(ZN(I,J),I=1,10),J=1,IGD)
      WRITE(3,911) (J,(ZN(I,J),I=11,16),J=1,IGD)
      DO 635 J=1,IGD
  635 ADV(J)=ZN(14,J)*(ZN(6,J)-AN)/(2.*CA*AN*ZN(6,J))
      WRITE(3,940) (J,ADV(J),J=1,IGD)
C
C     CALCULATE OBJ
C
      OBJ=-CT*((T1M-ZN(7,1))**2+(ZN(7,1)-ZN(8,1))**2)
      DO 640 J=1,IGD
      OBJ=OBJ+(C1*CQ*ZN(6,J)+C2*Q*ZN(3,J)+C3*Q*(1.-ZN(3,J)-ZN(4,J))
     1 -CI*(AIM-ZN(5,J))**2-CA*((ZN(14,J)*(ZN(6,J)-AN)*0.5)/
     2 (CA*AN))**2)*DT
  640 CONTINUE
      WRITE(3,935) OBJ
      IF(NO.EQ.13) GO TO 1111
      DO 650 J=1,IGD
      DO 650 I=1,M
  650 Z(I,J)=ZN(I,J)
C
C     SET LIMITS
C
      IF(Z(7,1).LT.300.) Z(7,1)=300.
      IF(Z(8,1).LT.300.) Z(8,1)=300.
      IF(Z(7,1).GT.370.) Z(7,1)=370.
      IF(Z(8,1).GT.370.) Z(8,1)=370.
      DO 660 J=1,IGD
      Z(7,J)=Z(7,1)
  660 Z(8,J)=Z(8,1)
      GO TO 15
C
C     FORMAT STATEMENT
```

```
C
  900 FORMAT(8F10.3)
  905 FORMAT(2D10.3,6F10.3)
  910 FORMAT(' STARTING APPROXIMATION',///,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  911 FORMAT(///,2X,'GD',7X,'Z11', 9X,'Z12', 9X,'Z13', 9X,'Z14', 9X,
     1 'Z15', 9X,'Z16',//,(I4,6F12.5))
  912 FORMAT(1H1,'NO. OF ITERATION=',I2)
  915 FORMAT(//////,' PARTICULAR SOLU',//,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  920 FORMAT(//////,' HOMOGENEOUS SOLU',I2,//,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  925 FORMAT(////, ' INTEGRATION CONSTANT',//,(10D12.4))
  930 FORMAT(////////, ' GENERAL SOLUTION',//,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  935 FORMAT(///,' O B J =',F13.6,/20(1H*))
  940 FORMAT(///,' ADVERTISMENT',/,(I4,5X,F12.5))
  945 FORMAT(1H0,'GA,GB,EA,EB,R,Q,V1,V2',//,2D10.3,6F10.3,//)
  950 FORMAT(1H0,'AIM,AN,CC,CT,T1M,X0,Y0,DT',//,8F10.5,//)
  955 FORMAT(1H0,'CQ,C1,C2,C3,CI,CA',//,8F10.5,//)
  970 FORMAT(8F10.5)
 1111 CONTINUE
      STOP
      END
```

```
      SUBROUTINE FFUNC(GA,GB,EA,EB,R,Q,V1,V2,AIM,AN,CC,CQ,C1,C2,C3,
     1 CI,CA,X0,Y0,Z,F)
C
C
C     THIS SUBROUTINE CALCULATES THE FUNCTIONAL VALUE OF THE
C     16 DIFFERENTIAL EQUATIONS
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Z(16),F(16)
      AT1=DEXP(-EA/(R*Z(7  )))*GA
      BT1=DEXP(-EB/(R*Z(7  )))*GB
      AT2=DEXP(-EA/(R*Z(8  )))*GA
      BT2=DEXP(-EB/(R*Z(8  )))*GB
      F(1)=Q/V1*(X0-Z(1))-AT1*Z(1)
      F(2)=Q/V1*(Y0-Z(2))-BT1*Z(2)+AT1*Z(1)
      F(3)=Q/V2*(Z(1)-Z(3))-AT2*Z(3)
      F(4)=Q/V2*(Z(2)-Z(4))-BT2*Z(4)+AT2*Z(3)
      F(5)=Q*Z(4)-Z(6)
      F(6)=(AN-Z(6))*(CC*Z(6)+Z(14)*(Z(6)-AN)/(2.*CA*AN))/AN
      F(7)=0.0
      F(8)=0.0
      F(9)=Q*(Z(9)/V1-Z(11)/V2)+(Z(9)-Z(10))*AT1
      F(10)=Q*(Z(10)/V1-Z(12)/V2)+Z(10)*BT1
      F(11)=Z(11)*Q/V2+(Z(11)-Z(12))*AT2+Q*(C2-C3)
      F(12)=Z(12)*Q/V2+Z(12)*BT2-Q*(C3+Z(13))
      F(13)=2.*CI*(AIM-Z(5))
      F(14)=C1*CQ+Z(13)-CC*Z(14)-Z(14)*Z(14)/(2.*CA*AN)+2.*CC*Z(6)*
     1 Z(14)/AN+Z(6)*Z(14)*Z(14)/(2.*CA*AN*AN)
      F(15)=AT1*Z(1)*(EA/(R*Z(7)*Z(7)))*(Z(9)-Z(10))+Z(10)*BT1*Z(2)*EB
     1 /(R*Z(7)*Z(7))
      F(16)=(Z(11)-Z(12))*AT2*Z(3)*EA/(R*Z(8)*Z(8))+Z(12)*Z(4)*BT2
     1 *EB/(R*Z(8)*Z(8))
      RETURN
      END
```

```
      SUBROUTINE RUNGK
C
C
C     RUNGE-KUTTA
C
C     THIS SUBROUTINE IS USED TC INTEGRATE  16 LINEARIZED
C     ECLATIONS SIMULTANEOUSLY
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION ZN(16, 51),J1(16,16),RM(4,16),RZ(16),B(16)
      DOUBLE PRECISION J1
      COMMON ZN,J1,RM,RZ,B,DT,M,N
      DO 10 MM=1,M
   10 RZ(MM)=ZN(MM,N)
      DO 40 L=1,4
      RM(L,1)=(J1(1,1)*RZ(1)+J1(1,7)*RZ(7)+B(1))*DT
      RM(L,2)=(J1(2,2)*RZ(2)+J1(2,1)*RZ(1)+J1(2,7)*RZ(7)+B(2))*DT
      RM(L,3)=(J1(3,1)*RZ(1)+J1(3,3)*RZ(3)+J1(3,8)*RZ(8)+B(3))*DT
      RM(L,4)=(J1(4,2)*RZ(2)+J1(4,3)*RZ(3)+J1(4,4)*RZ(4)+J1(4,8)*
     1 RZ(8)+B(4))*DT
      RM(L,5)=(J1(5,4)*RZ(4)+J1(5,6)*RZ(6)+B(5))*DT
      RM(L,6)=(J1(6,6)*RZ(6)+J1(6,14)*RZ(14)+B(6))*DT
      RM(L,7)=0.0
      RM(L,8)=0.0
      RM(L,9)=(J1(9,7)*RZ(7)+J1(9,9)*RZ(9)+J1(9,10)*RZ(10)+
     1 J1(9,11)*RZ(11)+B(9))*DT
      RM(L,10)=(J1(10,7)*RZ(7)+J1(10,10)*RZ(10)+J1(10,12)*RZ(12)+
     1 B(10))*DT
      RM(L,11)=(J1(11,8)*RZ(8)+J1(11,11)*RZ(11)+J1(11,12)*RZ(12)+
     1 B(11))*DT
      RM(L,12)=(J1(12,8)*RZ(8)+J1(12,12)*RZ(12)+J1(12,13)*RZ(13)+
     1 B(12))*DT
      RM(L,13)=(J1(13,5)*RZ(5)+B(13))*DT
      RM(L,14)=(J1(14,6)*RZ(6)+J1(14,13)*RZ(13)+J1(14,14)*RZ(14)+
     1 B(14))*DT
      RM(L,15)=(J1(15,1)*RZ(1)+J1(15,2)*RZ(2)+J1(15,7)*RZ(7)+
     1 J1(15,9)*RZ(9)+J1(15,10)*RZ(10)+B(15))*DT
      RM(L,16)=(J1(16,3)*RZ(3)+J1(16,4)*RZ(4)+J1(16,8)*RZ(8)+
     1 J1(16,11)*RZ(11)+J1(16,12)*RZ(12)+B(16))*DT
      AAA=0.5
      IF(L.EQ.3) AAA=1.
      DO 40 MM=1,M
      RZ(MM)=ZN(MM,N)+AAA*RM(L,MM)
   40 CONTINUE
      DO 50 I=1,M
   50 ZN(I,N+1)=ZN(I,N)+(RM(1,I)+2.*RM(2,I)+2.*RM(3,I)+RM(4,I))/6.
      RETURN
      END
```

```
C     ..................................................................
C
C        SUBROUTINE DGELG
C
C        PURPOSE
C           TO SOLVE A GENERAL SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS.
C           CALL DGELG(R,A,M,N,EPS,IER)
C
C        DESCRIPTION OF PARAMETERS
C           R      - DOUBLE PRECISION M BY N RIGHT HAND SIDE MATRIX
C                    (DESTROYED). ON RETURN R CONTAINS THE SOLUTIONS
C                    OF THE EQUATIONS.
C           A      - DOUBLE PRECISION M BY M COEFFICIENT MATRIX
C                    (DESTROYED).
C           M      - THE NUMBER OF EQUATIONS IN THE SYSTEM.
C           N      - THE NUMBER OF RIGHT HAND SIDE VECTORS.
C           EPS    - SINGLE PRECISION INPUT CONSTANT WHICH IS USED AS
C                    RELATIVE TOLERANCE FOR TEST ON LOSS OF
C                    SIGNIFICANCE.
C           IER    - RESULTING ERROR PARAMETER CODED AS FOLLOWS
C                    IER=0  - NO ERROR,
C                    IER=-1 - NO RESULT BECAUSE OF M LESS THAN 1 OR
C                             PIVOT ELEMENT AT ANY ELIMINATION STEP
C                             EQUAL TO 0,
C                    IER=K  - WARNING DUE TO POSSIBLE LOSS OF SIGNIFI-
C                             CANCE INDICATED AT ELIMINATION STEP K+1,
C                             WHERE PIVOT ELEMENT WAS LESS THAN OR
C                             EQUAL TO THE INTERNAL TOLERANCE EPS TIMES
C                             ABSOLUTELY GREATEST ELEMENT OF MATRIX A.
C
C        REMARKS
C           INPUT MATRICES R AND A ARE ASSUMED TO BE STORED COLUMNWISE
C           IN M*N RESP. M*M SUCCESSIVE STORAGE LOCATIONS. ON RETURN
C           SOLUTION MATRIX R IS STORED COLUMNWISE TOO.
C           THE PROCEDURE GIVES RESULTS IF THE NUMBER OF EQUATIONS M IS
C           GREATER THAN 0 AND PIVOT ELEMENTS AT ALL ELIMINATION STEPS
C           ARE DIFFERENT FROM 0. HOWEVER WARNING IER=K - IF GIVEN -
C           INDICATES POSSIBLE LOSS OF SIGNIFICANCE. IN CASE OF A WELL
C           SCALED MATRIX A AND APPROPRIATE TOLERANCE EPS, IER=K MAY BE
C           INTERPRETED THAT MATRIX A HAS THE RANK K. NO WARNING IS
C           GIVEN IN CASE M=1.
C
C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C           NONE
C
C        METHOD
C           SOLUTION IS DONE BY MEANS OF GAUSS-ELIMINATION WITH
C           COMPLETE PIVOTING.
C
C     ..................................................................
```

```
C
      SUBROUTINE DGELG(R,A,M,N,EPS,IER)
C
C
      DIMENSION A(1),R(1)
      DOUBLE PRECISION R,A,PIV,TB,TOL,PIVI,DABS,EPS
      IF(M)23,23,1
C
C     SEARCH FOR GREATEST ELEMENT IN MATRIX A
    1 IER=0
      PIV=0.D0
      MM=M*M
      NM=N*M
      DO 3 L=1,MM
      TB=DABS(A(L))
      IF(TB-PIV)3,3,2
    2 PIV=TB
      I=L
    3 CONTINUE
      TOL=EPS*PIV
C     A(I) IS PIVOT ELEMENT. PIV CONTAINS THE ABSOLUTE VALUE OF A(I).
C
C
C     START ELIMINATION LOOP
      LST=1
      DO 17 K=1,M
C
C     TEST ON SINGULARITY
      IF(PIV)23,23,4
    4 IF(IER)7,5,7
    5 IF(PIV-TOL)6,6,7
    6 IER=K-1
    7 PIVI=1.D0/A(I)
      J=(I-1)/M
      I=I-J*M-K
      J=J+1-K
C     I+K IS ROW-INDEX, J+K COLUMN-INDEX OF PIVOT ELEMENT
C
C     PIVOT ROW REDUCTION AND ROW INTERCHANGE IN RIGHT HAND SIDE R
      DO 8 L=K,NM,M
      LL=L+I
      TB=PIVI*R(LL)
      R(LL)=R(L)
    8 R(L)=TB
C
C     IS ELIMINATION TERMINATED
      IF(K-M)9,18,18
C
C     COLUMN INTERCHANGE IN MATRIX A
    9 LEND=LST+M-K
```

```
      IF(J)12,12,10
   10 II=J*M
      CO 11 L=LST,LEND
      TB=A(L)
      LL=L+II
      A(L)=A(LL)
   11 A(LL)=TB
C
C     ROW INTERCHANGE AND PIVOT ROW REDUCTION IN MATRIX A
   12 DO 13 L=LST,MM,M
      LL=L+I
      TB=PIVI*A(LL)
      A(LL)=A(L)
   13 A(L)=TB
C
C     SAVE COLUMN INTERCHANGE INFORMATION
      A(LST)=J
C
C     ELEMENT REDUCTION AND NEXT PIVOT SEARCH
      PIV=0.D0
      LST=LST+1
      J=0
      DO 16 II=LST,LEND
      PIVI=-A(II)
      IST=II+M
      J=J+1
      DO 15 L=IST,MM,M
      LL=L-J
      A(L)=A(L)+PIVI*A(LL)
      TB=DABS(A(L))
      IF(TB-PIV)15,15,14
   14 PIV=TB
      I=L
   15 CONTINUE
      DO 16 L=K,NM,M
      LL=L+J
   16 R(LL)=R(LL)+PIVI*R(L)
   17 LST=LST+M
C     END OF ELIMINATION LOOP
C
C
C     BACK SUBSTITUTION AND BACK INTERCHANGE
   18 IF(M-1)23,22,19
   19 IST=MM+M
      LST=M+1
      DO 21 I=2,M
      II=LST-I
      IST=IST-LST
      L=IST-M
      L=A(L)+.5D0
```

```
      DO 21 J=II,NM,M
      TB=R(J)
      LL=J
      DO 20 K=IST,MM,M
      LL=LL+1
   20 TB=TB-A(K)*R(LL)
      K=J+L
      R(J)=R(K)
   21 R(K)=TB
   22 RETURN
C
C
C     ERRCR RETURN
   23 IER=-1
      RETURN
      ENC
```

APPENDIX 2

COMPUTER PROGRAM USED IN CHAPTER 5

```
C
C      THESIS,PROBLEM 2
C
C      ONE REACTOR ONLY
C      THIS PROGRAM SOLVES A SET OF 12 DIFF. EQUATIONS TWO-POINT
C      SPLIT TYPE USING THE SUPERPOSITION PRINCIPLE AND RUNGE-
C      KUTTA TECHNIQUE
C
C
       IMPLICIT REAL*8(A-H,O-Z)
       DIMENSION Z(12, 51),X(12),FF(12, 51),ZN(12, 51),J1(12,12),
      1 B(12),ZP(12, 51),ZH(08,12, 51),ZFC(16),RZ(12),RM(4,12),F(12)
      2 ,A(196),ADV(51)
       DOUBLE PRECISION J1
       COMMON ZN,J1,RM,RZ,B,DT,M,N
C
C      READ IN DATA
C
       READ(1,905) GA,GB,EA,EB,R,Q
       READ(1,900) AIM,AN,CC,CT,T1M,XO,YO,DT
       READ(1,900) CQ,C1,C2,C3,CI,CA
       READ(1,901) AO,A1,A2,BC,B1,B2
C
C      ECHO CHECK
C
       WRITE(3,945) GA,GB,EA,EB,R,Q,V1,V2
       WRITE(3,950) AIM,AN,CC,CT,T1M,XO,YO,DT
       WRITE(3,955) CQ,C1,C2,C3,CI,CA
       WRITE(3,960) AO,A1,A2,BC,B1,B2
C
C
       NO=C
       M=12
       IGD=1./DT+1
       EPS=0.0000001
C
C      INITIAL APPROXIMATION
C
       DO 10 J=1,IGD
       Z(1,J)=0.43
       Z(2,J)=0.53
       Z(3,J)=340.
       Z(4,J)=10.
       Z(5,J)=4.
       Z(6,J)=4.
       Z(7,J)=-20.
       Z(8,J)=-40.
       Z(9,J)=0.0
       Z(10,J)=-0.1
       Z(11,J)=0.0
```

```
      Z(12,J)=0.0
   10 CCNTINUE
   15 CCNTINUE
      NO=NO+1
      WRITE(3,912) NO
      WRITE(3,910) (J,(Z(I,J),I=1,10),J=1,IGD,10)
      WRITE(3,911)(J,(Z(I,J),I=11, M),J=1,IGD,10)
      DC 50 J=1,IGD
      DO 20 I=1,M
   20 X(I)=Z(I,J)
      CALL FFUNC(GA,GB,EA,EB,R,C,       AIM,AN,CC,CQ,C1,C2,C3,CI,CA,
     1 XC,YO, X,F)
      DO 30 I=1,M
   30 FF(I,J)=F(I)
   50 CCNTINUE
C
C     PARTICULAR SOLUTICN
C
      MH=0
      ZN(1,1)=0.53
      ZN(2,1)=0.43
      ZN(3,1)=0.0
      ZN(4,1)=0.0
      ZN(5,1)=7.
      ZN(6,1)=0.1
      DO 60 I=7,M
   6C ZN(I,1)=0.0
  50C CCNTINUE
      DO 200 N=1,IGD
      AT1=DEXP(-EA/(R*Z(3,N)))*GA
      BT1=DEXP(-EB/(R*Z(3,N)))*GB
      AT11=EA/(R*Z(3,N)*Z(3,N))
      BT11=EB/(R*Z(3,N)*Z(3,N))
      V1=Z(4,N)
      V12=V1*V1
      J1(1,1)=-Q/V1-AT1
      J1(1,3)=-Z(1,N)*AT1*AT11
      J1(1,4)=-Q*(XO-Z(1,N))/V12
      J1(2,1)=AT1
      J1(2,2)=-Q/V1-BT1
      J1(2,3)=-Z(2,N)*BT1*BT11+Z(1,N)*AT1*AT11
      J1(2,4)=-Q*(YC-Z(2,N))/V12
      J1(5,2)=Q
      J1(5,6)=-1.
      J1(6,6)=CC-2.*Z(6,N)*CC/AN+Z(12,N)/(CA*AN)-Z(6,N)*Z(12,N)/
     1 (CA*AN*AN)
      J1(6,12)=Z(6,N)/(CA*AN)-1./(2.*CA)-Z(6,N)*Z(6,N)/(2.*CA*AN*AN)
      J1(7,3)=(Z(7,N)-Z(8,N))*AT1*AT11
      J1(7,4)=-Z(7,N)*Q/V12
      J1(7,7)=Q/V1+AT1
```

```
      J1(7,8)=-AT1
      J1(8,3)=Z(8,N)*BT1*BT11
      J1(8,4)=-Z(8,N)*Q/V12
      J1(8,8)=Q/V1+BT1
      J1(8,11)=-Q
      J1(9,1)=(Z(7,N)-Z(8,N))*AT1*AT11
      J1(9,2)=Z(8,N)*BT1*BT11
      J1(9,3)=(Z(7,N)-Z(8,N))*Z(1,N)*AT1*AT11*(AT11-2./Z(3,N))+
     1 Z(8,N)*Z(2,N)*BT1*BT11*(BT11-2./Z(3,N))
      J1(9,7)=Z(1,N)*AT1*AT11
      J1(9,8)=-Z(1,N)*AT1*AT11+Z(2,N)*BT1*BT11
      J1(10,1)=-Z(7,N)*Q/V12
      J1(10,2)=-Z(8,N)*Q/V12
      J1(10,4)=(Z(7,N)*(XO-Z(1,N))+Z(8,N)*(YO-Z(2,N)))*Q*(-2.)/(V1*V12)
      J1(10,7)=Q*(XO-Z(1,N))/V12
      J1(10,8)=Q*(YO-Z(2,N))/V12
      J1(11,5)=-2.*CI
      J1(12,6)=2.*CC*Z(12,N)/AN+Z(12,N)*Z(12,N)/(2.*CA*AN*AN)
      J1(12,11)=1.
      J1(12,12)=-CC-Z(12,N)/(CA*AN)+2.*CC*Z(6,N)/AN+Z(6,N)*Z(12,N)/
     1 (CA*AN*AN)
      IF(MH.NE.0) GO TO 110
      B(1)=-(J1(1,1)*Z(1,N)+J1(1,3)*Z(3,N)+J1(1,4)*Z(4,N))+FF(1,N)
      B(2)=-(J1(2,1)*Z(1,N)+J1(2,2)*Z(2,N)+J1(2,3)*Z(3,N)+J1(2,4)*
     1 Z(4,N))+FF(2,N)
      B(3)=0.0
      B(4)=0.0
      B(5)=-(J1(5,2)*Z(2,N)+J1(5,6)*Z(6,N))+FF(5,N)
      B(6)=-(J1(6,6)*Z(6,N)+J1(6,12)*Z(12,N))+FF(6,N)
      B(7)=-(J1(7,3)*Z(3,N)+J1(7,4)*Z(4,N)+J1(7,7)*Z(7,N)+J1(7,8)*
     1 Z(8,N))+FF(7,N)
      B(8)=-(J1(8,3)*Z(3,N)+J1(8,4)*Z(4,N)+J1(8,8)*Z(8,N)+J1(8,11)*
     1 Z(11,N))+FF(8,N)
      B(9)=-(J1(9,1)*Z(1,N)+J1(9,2)*Z(2,N)+J1(9,3)*Z(3,N)+J1(9,7)*
     1 Z(7,N)+J1(9,8)*Z(8,N))+FF(9,N)
      B(10)=-(J1(10,1)*Z(1,N)+J1(10,2)*Z(2,N)+J1(10,4)*Z(4,N)+J1(10,7)*
     1 Z(7,N)+J1(10,8)*Z(8,N))+FF(10,N)
      B(11)=-J1(11,5)*Z(5,N)+FF(11,N)
      B(12)=-(J1(12,6)*Z(6,N)+J1(12,12)*Z(12,N)+J1(12,11)*Z(11,N))+
     1 FF(12,N)
      GO TO 120
  110 DO 115 I=1,M
  115 B(I)=0.0
  120 CONTINUE
      CALL RUNGK
  200 CONTINUE
      IF(MH.NE.0) GO TO 300
      DO 220 J=1,IGD
      DO 220 I=1,M
      ZP(I,J)=ZN(I,J)
```

```
  220 CONTINUE
      WRITE(3,915)(J,(ZP(I,J),I=1,10),J=1,IGD,10)
      WRITE(3,911) (J,(ZP(I,J),I=11, M),J=1,IGC,10)
C
C     HOMOGENEOUS  SOLUTION
C
      MH=1
      DO 230 I=1,M
  230 ZN(I,1)=0.0
      ZN(3,1)=1.
      GO TO 500
  300 CONTINUE
      DO 350 J=1,IGD
      DO 350 I=1,M
  350 ZH(MH,I,J)=ZN(I,J)
      WRITE(3,920)MH,(J,(ZH(MH,I,J),I=1,10),J=1,IGD,10)
  630 WRITE(3,911) (J,(ZH(MH,I,J),I=11, M),J=1,IGD,10)
      GO TO (420,430,440,450,460,470,480,550),MH
  420 MH=2
      ZN(3,1)=0.0
      ZN(4,1)=1.0
      GO TO 500
  430 MH=3
      ZN(4,1)=0.0
      ZN(7,1)=1.0
      GO TO 500
  440 MH=4
      ZN(7,1)=0.0
      ZN(8,1)=1.0
      GO TO 500
  450 MH=5
      ZN(8,1)=0.0
      ZN(9,1)=1.0
      GO TO 500
  460 MH=6
      ZN(9,1)=0.0
      ZN(10,1)=1.0
      GO TO 500
  470 MH=7
      ZN(10,1)=0.0
      ZN(11,1)=1.0
      GO TO 500
  480 MH=8
      ZN(11,1)=0.0
      ZN(12,1)=1.0
      GO TO 500
  550 CONTINUE
C
C     BOUNDARY CONDITION
C
```

```
      DO 563 J=1,8
      DC 562 I=7,12
      II=I-6
  562 J1(II,J)=ZH(J,I,IGD)
      J1(7,J)=2.*CT*ZH(J,3,1)+ZH(J,9,1)
  563 J1(8,J)=2.*A2*ZH(J,4,1)+ZH(J,10,1)
      DO 570 I=7,12
      II=I-6
  570 B(II)=       -ZP(I,IGD)
      B(7)=2.*CT*(T1M-ZP(3,1))-ZP(9,1)
      B(8)=-A1-2.*A2*ZP(4,1)-ZP(10,1)
      DC 580 J=1,8
      DO 580 I=1,8
      II=(J-1)*8+I
  580 A(II)=J1(I,J)
      CALL DGELG(B,A, 8,1,EPS,IER)
      WRITE(3,925) (B(I),I=1, 8)
C
C     GENERAL SOLUTION
C
      DO 620 J=1,IGD
      DO 620 I=1,M
      S=0.0
      DO 610 L=1,8
  610 S=S+B(L)*ZH(L,I,J)
  620 ZN(I,J)=ZP(I,J)+S
C
C     PRINT OUT SOLUTIONS
C
      WRITE(3,930) (J,(ZN(I,J),I=1,10),J=1,IGD)
      WRITE(3,911) (J,(ZN(I,J),I=11, M),J=1,IGD)
      DO 635 J=1,IGD
  635 ADV(J)=ZN(12,J)*(ZN(6,J)-AN)/(2.*CA*AN*ZN(6,J))
      WRITE(3,940) (J,ADV(J),J=1,IGD)
C
C     CALCULATE OBJ
C
      OBJ=-CT* (T1M-ZN(3,1))**2
     1 -(AC+A1*ZN( 4,1)+A2*ZN( 4,1)*ZN( 4,1))
      DO 640 J=1,IGD
      OBJ=OBJ+(C1*CQ*ZN(6,J)+C2*Q*ZN(1,J)+C3*Q*(1.-ZN(1,J)-ZN(2,J))
     1 -CI*(AIM-ZN(5,J))**2-CA*ADV(J)**2*ZN(6,J)**2)*DT
  640 CONTINUE
      WRITE(3,935) OBJ
      IF(NO.EQ.17) GO TO 1111
      DO 650 J=1,IGD
      DO 650 I=1,M
  650 Z(I,J)=ZN(I,J)
C
C     SET LIMITS
```

```
C
      IF(Z(3,1).LT.300.) Z(3,1)=300.
      IF(Z(3,1).GT.390.) Z(3,1)=390.
      DO 660 J=1,IGD
      Z(3,J)=Z(3,1)
  660 CONTINUE
      DO 661 J=1,IGD
      IF(Z(1,J).LT.0.) Z(1,J)=0.0
  661 IF(Z(2,J).GT.1.) Z(2,J)=1.
      GO TO 15
C
C     FORMAT STATEMENT
C
  900 FORMAT(8F10.3)
  901 FORMAT(8F10.6)
  905 FORMAT(2D10.3,6F10.3)
  910 FORMAT(' STARTING APPROXIMATION',///,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  911 FORMAT(///,2X,'GD',7X,'Z11', 9X,'Z12',//,
     1 (I4,2F12.5))
  912 FORMAT(1H1,'NO. OF ITERATION=',I2)
  915 FORMAT(//////,' PARTICULAR SOLU',//,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  920 FORMAT(//////,' HOMOGENEOUS SOLU',I2,//,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  925 FORMAT(////, ' INTEGRATION CONSTANT',//,(10D12.4))
  930 FORMAT(////////, ' GENERAL SOLUTION',//,
     1 2X,'GD',7X,'Z1',10X,'Z2',10X,'Z3',10X,'Z4',10X,'Z5',10X,'Z6',
     2 10X,'Z7',10X,'Z8',10X,'Z9',10X,'Z10',//,(I4,10F12.5))
  935 FORMAT(///,' O B J =',F13.6,/20(1H*))
  940 FORMAT(///,' ADVERTISMENT',/,(I4,5X,F12.5))
  945 FORMAT(1H0,'GA,GB,EA,EB,R,Q,V1,V2',//,2D10.3,6F10.3,//)
  950 FORMAT(1H0,'AIM,AN,CC,CT,T1M,X0,Y0,DT',//,8F10.5,//)
  955 FORMAT(1H0,'C0,C1,C2,C3,CI,CA',//,8F10.5,//)
  960 FORMAT(1H0,'A0,A1,A2,B0,B1,B2',//,8F10.6,//)
 1111 STOP
      END
```

```
      SUBROUTINE FFUNC(GA,GB,EA,EB,R,Q,       AIM,AN,CC,CQ,C1,C2,C3,
     1 CI,CA,XO,YO,Z,F)
C
C
C     THIS SUBROUTINE CALCULATES THE FUNCTIONAL VALUE OF THE
C     12 DIFFERENTIAL EQUATIONS
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Z(12),F(12)
      V1=Z(4)
      AT1=DEXP(-EA/(R*Z(3)))*GA
      BT1=DEXP(-EB/(R*Z(3)))*GB
      F(1)=Q/V1*(XO-Z(1))-AT1*Z(1)
      F(2)=Q/V1*(YO-Z(2))-BT1*Z(2)+AT1*Z(1)
      F(3)=0.0
      F(4)=0.0
      F(5)=Q*Z(2)-Z(6)
      F(6)=(AN-Z(6))*(CC*Z(6)+Z(12)*(Z(6)-AN)/(2.*CA*AN))/AN
      F(7)=Z(7)*Q/V1+(Z(7)-Z(8))*AT1+Q*(C2-C3)
      F(8)=Z(8)*Q/V1+Z(8)*BT1-Q*(Z(11)-C3)
      F(9)=(Z(7)-Z(8))*AT1*Z(1)*EA/(R*Z(3)*Z(3))+Z(8)*BT1*Z(2)*EB/
     1 (R*Z(3)*Z(3))
      F(10)=Z(7)*Q*(XO-Z(1))/V1**2+Z(8)*Q*(YO-Z(2))/V1**2
      F(11)=2.*CI*(AIM-Z(5))
      F(12)=C1*CQ+Z(11)-CC*Z(12)-Z(12)*Z(12)/(2.*CA*AN)+2.*CC*Z(6)*
     1 Z(12)/AN+Z(6)*Z(12)*Z(12)/(2.*CA*AN*AN)
      RETURN
      END
```

```
      SUBROUTINE RUNGK
C
C
C     RUNGE-KUTTA
C
C     THIS SUBROUTINE IS USED TC INTEGRATE  12 LINEARIZED
C     EQUATIONS SIMULTANEOUSLY
C
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION ZN(12, 51),J1(12,12),RM(4,12),RZ(12),B(12)
      DOUBLE PRECISION J1
      COMMON ZN,J1,RM,RZ,B,DT,M,N
      DO 10 MM=1,M
   10 RZ(MM)=ZN(MM,N)
      DO 40 L=1,4
      RM(L,1)=(J1(1,1)*RZ(1)+J1(1,3)*RZ(3)+J1(1,4)*RZ(4)+B(1))*DT
      RM(L,2)=(J1(2,1)*RZ(1)+J1(2,2)*RZ(2)+J1(2,3)*RZ(3)+J1(2,4)*
     1 RZ(4)+B(2))*DT
      RM(L,3)=0.0
      RM(L,4)=0.0
      RM(L,5)=(J1(5,2)*RZ(2)+J1(5,6)*RZ(6)+B(5))*DT
      RM(L,6)=(J1(6,6)*RZ(6)+J1(6,12)*RZ(12)+B(6))*DT
      RM(L,7)=(J1(7,3)*RZ(3)+J1(7,4)*RZ(4)+J1(7,7)*RZ(7)+J1(7,8)*RZ(8)
     1 +B(7))*DT
      RM(L,8)=(J1(8,3)*RZ(3)+J1(8,4)*RZ(4)+J1(8,8)*RZ(8)+J1(8,11)*RZ(11)
     1 +B(8))*DT
      RM(L,9)=(J1(9,1)*RZ(1)+J1(9,2)*RZ(2)+J1(9,3)*RZ(3)+J1(9,7)*
     1 RZ(7)+J1(9,8)*RZ(8)+B(9))*DT
      RM(L,10)=(J1(10,1)*RZ(1)+J1(10,2)*RZ(2)+J1(10,4)*RZ(4)+J1(10,7)
     1 *RZ(7)+J1(10,8)*RZ(8)+B(10))*DT
      RM(L,11)=(J1(11,5)*RZ(5)+B(11))*DT
      RM(L,12)=(J1(12,6)*RZ(6)+J1(12,11)*RZ(11)+J1(12,12)*
     1 RZ(12)+B(12))*DT
      AAA=0.5
      IF(L.EQ.3) AAA=1.
      DO 40 MM=1,M
      RZ(MM)=ZN(MM,N)+AAA*RM(L,MM)
   40 CONTINUE
      DO 50 I=1,M
   50 ZN(I,N+1)=ZN(I,N)+(RM(1,I)+2.*RM(2,I)+2.*RM(3,I)+RM(4,I))/6.
      RETURN
      END
```

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QUASILINEARIZATION APPLIED TO NONLINEAR
BOUNDARY-VALUE PROBLEMS IN
OPTIMAL MANAGEMENT SYSTEMS

by

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ABSTRACT

In recent years, various techniques have been developed for seeking optimal design and operating policies of dynamic industrial management systems. However, each of these techniques has its own drawbacks. Methods such as calculus of variations and maximum principle are usually limited by the boundary-value difficulty in obtaining numerical solutions. Quasilinearization has been shown to be an effective tool for handling boundary-value problem. Thus the combined use of calculus of variations and quasilinearization can avoid this difficulty in seeking the numerical solutions of optimization problems.

The purpose of this thesis is to show that the quasilinearization technique can be used to find solutions of large dimensional optimization problems with the presence of unknown parameters. First, a complex production planning, advertising, and inventory system was optimized. In this problem, the temperatures in the chemical reactors are considered as the unknown parameters. Then a similar problem was solved with both the temperature and the volume of the reactor as the unknown parameters.

The results of the first problem indicate that considering temperature as a constant parameter is superior to considering it as a function of time. In practical applications, constant temperature is much easier to maintain than variable temperature. Furthermore, the results in this work show that the increasing

profit due to the use of variable temperature is very small. The results obtained for the second problem indicate that only one of the two reactors which was used in the first problem is needed. Having one big reactor whose volume is approximally equal to the sum of the two reactors produces approximately the same results as that of using two separate reactors. For both of the two problems, the additional unknown parameters do not significantly increase the amount of computation.