Optimal Control of a Distributed Parameter System.

Ahmad Shariat
Louisiana State University and Agricultural & Mechanical College

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in

The Department of Chemical Engineering

by

Ahmad Shariat
B.S., Tennessee Technological University, 1967
M.S., Louisiana State University, 1970
December, 1971
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ABSTRACT

The optimal control of chemical processes governed by a system of simultaneous partial differential equations was considered. The maximum principle for distributed parameter systems using the variational technique was derived for the system under consideration. By using a gradient technique the theory was applied to the optimal control of a plug-flow tubular reactor with nonlinear chemical kinetics.

The frequency response of system was obtained and was used to find approximate transfer functions. The theory of optimal control for the lumped parameter systems was applied to the system described by the approximate transfer functions to calculate a sub-optimal feedforward control. The yield obtained with this sub-optimal control agrees favorably with that obtained using the optimal control.

Optimal feedback control of the reactor was also considered. Using a direct search technique the optimal feedback control was obtained and compared to that of the optimal feedforward control. Comparable yields were obtained.
CHAPTER I
INTRODUCTION

A. Description of the Problem

The transient behavior of many systems of interest in applied engineering, such as chemical processes, aerospace systems, communications systems, thermal process, etc. are governed by systems of partial differential equations. The general practice in designing the optimal control of such systems has been to approximate the distributed parameter systems with lumped parameter systems, which are governed by systems of ordinary differential equations, and to apply the well developed theory of optimal control for lumped parameter systems.

In many instances approximating the distributed parameter systems (DPS) by lumped parameter systems does not produce as satisfactory an optimal control as would have been realized had the original distributive nature of the system been taken into consideration. Therefore, the need for the development of an optimum control theory for DPS was obvious. Within the last ten years considerable advances have been made in the development of both theory and application in this area. However, most of the work has been devoted to simple classes of DPS which have analytical solutions and consequently are of little importance to actual processes having no analytical solutions. Direct application of the optimal control theory of DPS has not been widely used due to mathematical complexities and computational difficulties in the solution, and unfamiliarity with the techniques.
The present work is concerned with the optimization and optimal control of a chemical reactor, whose dynamics are described by a set of three simultaneous partial differential equations in two independent variables.

B. Literature Review

The development of optimal control theory of DPS has paralleled that of lumped systems and is based upon state space modeling, optimal techniques, stability concepts, estimation problems, computational methods, and approximation techniques (3).

The work in optimal control theory of DPS was initiated in 1960 by Butkovskii and Lerner (15). They considered the formulation of the problem and designed a specific control system. Following this work, Butkovskii (11) (12) (13) developed a maximum principle for DPS which was analogous to the Pontryagin's maximum principle for lumped parameter systems. He considered systems whose dynamics were described by nonlinear integral equations. The difficulties in applying Butkovskii's maximum principle are: 1) the state variables must be in the form of integral equations, 2) it requires the explicit solution of the systems equation, thus restricting the results to linear systems, 3) the optimal control obtained is in the form of the solution of a nonlinear integral equation involving multiple integrals (such an integral equation is not soluble in general), and 4) state dependent constraints are difficult to include in the optimal solution. To overcome these difficulties, Butkoskii suggested spatial-discretization of DPS followed by the application of optimal control theory for lumped parameter systems.
to the approximate system. He also developed the method of moments (14) which requires the knowledge of the eigen functions of the DPS.

The deficiencies in Butkovskii's formulation were removed by Katz (32) who formulated a general maximum principle which did not require the integral representation of the state variables and could be applied to first order parabolic and hyperbolic systems, as well as lumped parameter systems.

Wang and Tung (77) presented a general view of the optimum control of DPS and discussed mathematical formulation, controllability and observability, derivation of a maximum principle for a particular system using dynamic programming and problems associated with approximation and discretization of DPS. Wang (73) also applied dynamic programming to a linear DPS with quadratic performance index to obtain the optimum control for a DPS with time delays. Egorov (24) obtained necessary conditions for the optimal control of a DPS which was described by partial differential equations of the second order. Senin (65) (66) considered statistical problems associated with DPS.

Adbikerimov (1) treated optimal control of discrete distributed systems and stated the necessary conditions. Sirazatinov (70) applied a combination of dynamic programming and the theory of the stability of processes with distributed systems, to investigate the optimal control and stability of DPS. Butkovskii and Poltavskii (16) (17) obtained optimal control of a distributed oscillatory system by using the method of moments and variational techniques.

Sakawa (60) used variational techniques to obtain the necessary
and sufficient conditions for the optimal control of one dimensional linear stationary DPS.

Wang (75) considered asymptotic stability of DPS with feedback control; sufficient conditions for Lyapunov asymptotic stability were derived for DPS and systems with time delay. He also discussed (76) a method to obtain a completely stable control law for systems described by parabolic and hyperbolic partial differential equations. Stability conditions for a class of nonlinear DPS were also derived by Blodgett (7) by generalization of Lyapunov's direct method; the results were applied to a chemical reactor process.

Vostrova (71) investigated sampled-data systems with distributed parameter elements. Denn, Gray, and Ferron (23) obtained necessary conditions for the optimal control of DPS by solving the linearized variational equations by Green's functions. The results were applied to optimal heat removal in a reactor with radial diffusion. An optimum boundary control was obtained by Kim and Erzberger (36) by applying dynamic programming to obtain Hamilton-Jacobi type equations for distributed systems.

Khatri (35) derived a necessary condition for the optimum control of a linear system with input delay or transportation lag. Degtyarev and Sirazedtdinov (20) considered optimum control of one-dimensional distributed processes described by a set of first order partial differential equations.

Kastenberg (31), by using the method of comparison functions, obtained a sufficient condition for global asymptotic stability of a particular class of distributed parameter feedback control systems. Brogan (9) showed that the dynamic programming approach
the maximum principle was just as powerful as variational techniques. Denn (22) considered a linear DPS and obtained the optimal controller for the system.

Koppel (43) derived time optimal control of a class of DPS. Koppel and Shih (45) reduced the solution of optimal control problem of a DPS to the solution of an analogous lumped-parameter system. Seinfeld and Lapidus (63) considered the computational aspects of finding optimal control of DPS and compared using the results from a method of steepest ascent and that of a direct search on the cost function. They also discussed (64) singular solutions in the optimal control of DPS.

Athans (3) defined and classified the optimal control of DPS and stated the requirements for a good control of DPS in comparison with that of lumped parameter systems. A new definition of observability for DPS was introduced by Goodson and Klein (27). Optimal control of DPS with constrained inputs was considered by Weigand and D'Souza (78) using a set of linear partial differential equations.

Wismer (80) introduced an efficient computational technique for obtaining the optimal control of a DPS which was defined by a vector parabolic partial differential equation. Time optimal control of a class of linear DPS was obtained by Lim (48). Shih (67) derived a necessary condition for the optimal control of a DPS with integral equation constraints. Herget (28) obtained conditions for null controllability of a linear DPS with constrained control input.
B. Purpose of the Investigation

This research is an attempt to obtain the optimal feedforward and feedback control of a system frequently found in chemical conversion processes. The system of interest is a jacketed tubular reactor in which the first-order reactions \[ K_1 A \rightarrow B \rightarrow K_2 C, \] where B is the desired product take place. The control is achieved by the manipulation of cooling water temperature.
A. **Formulation of the Problem**

In this chapter the mathematical definitions and the derivation of the maximum principle for distributed parameter systems (DPS) will be discussed. The definitions are based on the notations used by Wang (74); the maximum principle derivation for the DPS are based upon the derivation by Sage (58).

Let a DPS be defined in \( \mathbb{T} \times \Omega \), where \( \mathbb{T} \) is the time domain, and \( \Omega \) is an open, connected subset of an \( M \)-dimensional Euclidean space, \( E_M \), which denotes the spatial domain. The boundary of \( \Omega \) is defined by \( \partial \Omega \).

At any time \( t \in \mathbb{T} \), the state of a DPS is defined by a set of state vector functions \( \{X_i(t, \tilde{Z}), i = 1, \ldots, N\} \) for all \( \tilde{Z} \in \Omega \), where \( \tilde{Z} = \text{col}[Z_1, Z_2, \ldots, Z_m] \). The control of the DPS is achieved by applying the control function inputs \( \{U_j(t, \tilde{Z}), j = 1, \ldots, R\} \) to the system, which may run over the whole of the spatial domain \( \Omega \) or certain subsets of \( \Omega \).

The dynamics of a DPS are governed by a system of partial differential equations (PDE) of the form:

\[
\frac{\partial^n}{\partial t^n} X_i(t, \tilde{Z}) = F_i \left[ t, \tilde{Z}, \frac{\partial X_i(t, \tilde{Z})}{\partial \tilde{Z}}, \ldots, \frac{\partial^K X_i(t, \tilde{Z})}{\partial \tilde{Z}_1^K \ldots \partial \tilde{Z}_M^K}, \ldots, \tilde{U}(t, \tilde{Z}) \right]
\]

(2-1A)
where

\[ i = 1, \ldots, N \]

\[ M \]

\[ K = \sum_{i=0}^{M} K_i \leq n \]

In Equation (2-1A) \( n \) is the order of the \( i^{th} \) equation; which is the highest order time derivative in the \( i^{th} \) equation.

It is always possible to reduce the order of a differential equation by introducing new variables which correspond to the derivatives in the differential equation. Define the new variables as

\[ x_{10}(t, \tilde{z}) = x_1'(t, \tilde{z}), \quad x_{11}(t, \tilde{z}) = \frac{\partial}{\partial t} x_1'(t, \tilde{z}), \ldots, x_{1n-1} = \frac{\partial^{n-1}}{\partial t^{n-1}} x_1'(t, \tilde{z}) \]

\[ x_{N0}(t, \tilde{z}) = x_N'(t, \tilde{z}), \quad x_{N1}(t, \tilde{z}) = \frac{\partial}{\partial t} x_N'(t, \tilde{z}), \ldots, x_{Nn-1} = \frac{\partial^{n-1}}{\partial t^{n-1}} x_N'(t, \tilde{z}) \]

substituting these new variables in Equation (2-1A) reduces the PDE to a set of PDE which are first order with respect to time and have the general form of

\[ \frac{\partial \bar{x}(t, \tilde{z})}{\partial t} = K^T \left[ \frac{\partial \bar{x}(t, \tilde{z})}{\partial \tilde{z}}, \ldots, \frac{\partial^{K_i} \bar{x}(t, \tilde{z})}{\partial z_1^{K_{i1}} \ldots \partial z_M^{K_{iM}}} \right] (2-1B) \]

where

\[ K = \sum_{i=1}^{M} K_i \]

It is also possible to reduce the order of spatial derivatives by introducing new variables, but from the dynamic and state representation point of view this is not desirable. For notational simplicity define
substitution in Equation (2-1B) results in

\[
\frac{\partial^K \bar{x}(t,\tilde{z})}{\partial \tilde{z}^K} \Delta \frac{\partial^K \bar{x}(t,\tilde{z})}{\partial z_1 \partial z_2 \ldots \partial z_M}, \quad K = \sum_{i=1}^{M} i
\]

The vector function \( \bar{F} \) is an \( N \)-dimensional vector defined in \( \tau \times \Omega \) and is assumed to be at least twice piecewise continuously differentiable with respect to its arguments.

The problem of the optimum control of a DPS is to determine a control vector subject to certain constraints, such that when it is applied to the system, a given performance index is minimized (maximized). Therefore, the problem could be stated as, given the system of PDE (2-1) with the initial condition

\[
\tilde{x}(t_0,\tilde{z}) = x_0(\tilde{z}) \quad (2-2)
\]

and the boundary condition

\[
\frac{\partial^{K-1} \tilde{x}(t,\tilde{z})}{\partial \tilde{z}^{K-1}} \bigg|_{\partial \Omega} = c_1; \quad \frac{\partial^{K-2} \tilde{x}(t,\tilde{z})}{\partial \tilde{z}^{K-2}} \bigg|_{\partial \Omega} = c_2; \ldots ; \frac{\partial \tilde{x}(t,\tilde{z})}{\partial \tilde{z}} \bigg|_{\partial \Omega} = c_{K-1} \quad (2-3)
\]

where \( c_1, c_2, \ldots, c_{K-1} \) are given constants, it is required to find a bounded piecewise continuous control vector \( \tilde{U}(t,\tilde{z}) \) where

\[
\tilde{U}(t,\tilde{z}) \in \omega \text{ and } \omega \text{ is a set defined by}
\]

\[
\omega[\tilde{U}(t,\tilde{z}) \mid g_i(\tilde{U}(t,\tilde{z})) \leq M_i \text{ } \forall i = 1, \ldots, Q \leq R \quad (2-4)
\]
where $M_i$'s are defined constants; such that a prescribed performance index of Mayer-Bolza form:

$$J = \int_{t_0}^{t_f} \int_{\Omega} \theta[\bar{X}(t, \bar{Z}), t_f] d\Omega + \int_{t_0}^{t_f} \int_{\Omega} \varphi(t, \bar{Z}, \bar{X}(t, \bar{Z}), \frac{\partial K_{\bar{Z}}(t, \bar{Z})}{\partial \bar{Z}}, \bar{u}(t, \bar{Z}) d\Omega dt$$

(2-5)

where $\theta$ and $\varphi$ are scalar functions of the vector variables, $t_0$ and $t_f$ are specified initial and final time, is minimized. Any control $\bar{u}(t, \bar{Z})$ which satisfies Equation (2-4) is called an admissible control.

It is also assumed that the problem is well posed, i.e., its solution exists, is unique, and depends continuously on the initial state. If maximization of $J$ is desired, it could be achieved by minimizing $-J$. Therefore, only minimization will be considered.

B. Maximum Principle for DPS

Let $\bar{U}^*(t, \bar{Z})$ be the desired solution for the DPS. Then application of this control vector to the system would result in a trajectory $\bar{X}^*(t, \bar{Z})$ which is called the optimal trajectory. Using $\bar{U}^*(t, \bar{Z})$ and $\bar{X}^*(t, \bar{Z})$ to evaluate $J$ results in an optimal $J$ which is denoted by $J^*$. For notational simplicity the arguments of the vectors will be dropped unless there is danger of ambiguity.

Now, consider a control vector $\tilde{U}$ slightly different from the optimal control $U^*$. Application of this $\tilde{U}$ to the system (2-1) would result in a trajectory $\tilde{X}$ which is slightly different from $X^*$, or

$$\tilde{U}(t, \bar{Z}) = U^*(t, \bar{Z}) + \delta \tilde{U}(t, \bar{Z})$$

(2-6)

and

$$\tilde{X}(t, \bar{Z}) = \bar{X}^*(t, \bar{Z}) + \delta \bar{X}(t, \bar{Z})$$

(2-7)
where $\delta \bar{U}$ and $\delta \bar{X}$ are variations in $\bar{U}$ and $\bar{X}$ respectively. Corresponding to these new values of $\bar{U}$ and $\bar{X}$ there is a new value of $J$ which is different from $J^*$ by

$$J = J^* + \delta J \quad (2-8)$$

If $J$ is an optimal value, then $\delta J$ must be zero, since it was assumed the solution was unique. Therefore, if one substitutes Equations (2-6), (2-7), and (2-8) into Equation (2-5) and finds the variation, $\delta J$ of $J$, equating this to zero results in the necessary conditions for optimality.

As for the optimal control of a lumped parameter system, define the Hamiltonian $H$ for the DPS as

$$H = \left[ t, \bar{Z}, \bar{X}(t, \bar{Z}), \frac{\partial K}{\partial Z_k(t, \bar{Z})}, U(t, \bar{Z}), P(t, \bar{Z}) \right] =$$

$$= \varphi \left[ t, \bar{Z}, \bar{X}(t, \bar{Z}), \frac{\partial K}{\partial Z_k(t, \bar{Z})}, U(t, \bar{Z}) \right] + P^T(t, \bar{Z}) \left[ \bar{P}(t, \bar{Z}), \bar{X}(t, \bar{Z}), \frac{\partial K}{\partial Z_k(t, \bar{Z})}, \bar{U}(t, \bar{Z}) \right] \quad (2-9)$$

where $P^T(t, \bar{Z})$ is the transpose of an $-N$ dimensional adjoint vector which must be found. From Equations (2-9) and (2-1) one obtains

$$\varphi = H - P^T \frac{\partial \bar{X}}{\partial T} \quad (2-10)$$

Substituting the above into Equation 2-5 results in

$$J = \int_0^{\Omega} \theta \, dt + \int_{t_f}^{t_o} \left[ H - P^T \frac{\partial \bar{X}}{\partial T} \right] \, dt \quad (2-11)$$
Now, one obtains the first variation of $J$ due to variation of $\tilde{U}$ as

$$\delta J = \int_\Omega \delta \mathbf{x} (t, \tilde{Z}) \frac{\partial F}{\partial \mathbf{x}} \, d\Omega + \int_0^T \int_\Omega \left\{ (\delta \mathbf{x})^T \frac{\partial H}{\partial \mathbf{x}} + \left[ \delta \left( \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K} \right) \right]^T \frac{\partial H}{\partial \mathbf{z}^K} \right\} \, d\Omega dt$$

$$+ \left( \delta \tilde{U} \right)^T \frac{\partial H}{\partial \tilde{U}} - \left( \delta \tilde{U} \right)^T \left( \frac{\partial (\delta \tilde{X})}{\partial T} \right) \right\} \, d\Omega dt \tag{2.12}$$

Since, the $\delta$ operator and the derivative operator are interchangeable, one could write

$$\left[ \delta \left( \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K} \right) \right]^T \frac{\partial H}{\partial \left[ \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K} \right]} = \left[ \frac{\partial \mathbf{X}^K (\delta \mathbf{x})}{\partial \mathbf{z}^K} \right]^T \frac{\partial H}{\partial \mathbf{z}^K} \tag{2.13}$$

Equation (2.13) is expanded using the following identity:

$$\frac{d^n W}{dt^n} \mathbf{v} = \frac{d}{dt} \left( \frac{d^{n-1} W}{dt^{n-1}} \mathbf{v} \right) - \left( \frac{d^{n-1} W}{dt^{n-1}} \frac{dv}{dt} \right) \tag{2.14}$$

then

$$\left[ \frac{\partial \mathbf{X}^K (\delta \mathbf{x})}{\partial \mathbf{z}^K} \right]^T \frac{\partial H}{\partial \left[ \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K} \right]} = \left( \frac{\partial}{\partial \mathbf{z}^K} \right)^T \left[ \left( \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K} \right) \frac{\partial H}{\partial \mathbf{z}^K} \right]$$

$$- \left( \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K-1} \right) \frac{\partial}{\partial \mathbf{z}^K} \left( \frac{\partial H}{\partial \mathbf{z}^K} \right) \tag{2.15}$$

Similarly the second term of Equation (2.15) may be expanded, if the process is continued and the results are substituted back in (2.15), one obtains

$$\left[ \frac{\partial \mathbf{X}^K (\delta \mathbf{x})}{\partial \mathbf{z}^K} \right]^T \frac{\partial H}{\partial \left[ \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K} \right]} = \Lambda + (-1)^{K-1} \left( \frac{\partial}{\partial \mathbf{z}^K} \right)^T \left\{ (\delta \mathbf{x}) \frac{\partial \mathbf{X}^K}{\partial \mathbf{z}^K-1} \frac{\partial H}{\partial \mathbf{z}^K} \right\}$$
\[ + (-1)^K \left\{ (\delta \vec{x})^T \frac{\partial^K}{\partial \vec{z}^K} \frac{\partial H}{\partial [\frac{\partial \vec{x}}{\partial \vec{z}^K}]} \right\} \]  
\[ \text{(2-16)} \]

where

\[ \Lambda = \left( \frac{\partial}{\partial \vec{z}} \right)^T \left\{ \frac{\partial^{K-1}(\delta \vec{x})}{\partial \vec{z}^{K-1}} \frac{\partial H}{\partial [\frac{\partial \vec{x}}{\partial \vec{z}^{K-1}}]} \right\} - \left( \frac{\partial}{\partial \vec{z}} \right)^T \left\{ \frac{\partial^{K-2}(\delta \vec{x})}{\partial \vec{z}^{K-2}} \frac{\partial H}{\partial [\frac{\partial \vec{x}}{\partial \vec{z}^{K-2}}]} \right\} + \left( \frac{\partial}{\partial \vec{z}} \right)^T \left\{ \frac{\partial^{K-3}(\delta \vec{x})}{\partial \vec{z}^{K-3}} \frac{\partial H}{\partial [\frac{\partial \vec{x}}{\partial \vec{z}^{K-3}}]} \right\} \ldots . \]  
\[ \text{(2-17)} \]

Equation (2-16) is substituted in (2-12)

\[ \delta J = \int \frac{\partial (\delta \vec{x})}{\partial t} \frac{\partial H}{\partial \vec{z}} - \frac{\partial (\delta \vec{x})}{\partial t} \frac{\partial H}{\partial \vec{z}} \left[ \frac{\partial^{K-1}}{\partial \vec{z}^{K-1}} \frac{\partial H}{\partial [\frac{\partial \vec{x}}{\partial \vec{z}^{K-1}}]} \right] \frac{\partial H}{\partial \vec{z}} \]  
\[ + (-1)^K \left\{ (\delta \vec{x})^T \frac{\partial^K}{\partial \vec{z}^K} \frac{\partial H}{\partial [\frac{\partial \vec{x}}{\partial \vec{z}^K}]} \right\} \]  
\[ \text{d} \Omega \text{d} t \]  
\[ \text{(2-18)} \]

but

\[ \frac{\partial (\delta \vec{x})}{\partial t} = \frac{\partial}{\partial t} [ (\delta \vec{x})^T \vec{F} ] - (\delta \vec{x})^T \frac{\partial \vec{F}}{\partial t} \]  
\[ \text{(2-19)} \]

and

\[ \int_{t_0}^{t_f} \int_{\Omega} \frac{\partial (\delta \vec{x})}{\partial t} \frac{\partial^K}{\partial \vec{z}^K} \frac{\partial H}{\partial [\frac{\partial \vec{x}}{\partial \vec{z}^K}]} \text{d} \Omega \text{d} t = \int_{t_0}^{t_f} \int_{\Omega} \left[ \frac{\partial}{\partial t} [ (\delta \vec{x})^T \vec{F} ] - (\delta \vec{x})^T \frac{\partial \vec{F}}{\partial t} \right] \text{d} \Omega \text{d} t \]
\[
\delta J = \int_{\Omega} \left[ \delta \bar{x}(t, \bar{z}) \bar{P}(t, \bar{z}) - \delta \bar{x}(t, \bar{z}) \bar{P}(t, \bar{z}) \right] \, d\Omega
\]

\[
- \int_{t_o}^{t_f} \int_{\Omega} (\delta \bar{x})^T \frac{\partial \bar{P}}{\partial t} \, d\Omega dt \quad (2-20)
\]

Since, the initial condition of \( \bar{x}(t_o, \bar{z}) \) is specified then \( \delta \bar{x}(t_o, \bar{z}) \) is equal to zero and Equation (2-20) is reduced to

\[
\int_{t_o}^{t_f} \int_{\Omega} \bar{P}^T \frac{\partial (\delta \bar{x})}{\partial t} \, d\Omega dt = \int_{\Omega} \delta \bar{x}^T(t_f, \bar{z}) \bar{P}(t_f, \bar{z}) \, d\Omega - \int_{t_o}^{t_f} \int_{\Omega} (\delta \bar{x}^T) \frac{\partial \bar{P}}{\partial t} \, d\Omega dt \quad (2-21)
\]

Equation (2-21) is substituted in (2-18)

\[
\delta J = \int_{\Omega} \delta \bar{x}^T(t_f, \bar{z}) \frac{\partial \theta_f}{\partial \bar{x}} \, d\Omega - \int_{\Omega} \delta \bar{x}^T(t_f, \bar{z}) \bar{P}(t_f, \bar{z}) \, d\Omega + \int_{t_o}^{t_f} \int_{\Omega} \left[ \delta \bar{x}^T \left( \sum_{j=1}^{K} \left( \frac{\partial H}{\partial \bar{x}^j} \right) \right) \right] \, d\Omega dt
\]

\[
+ \delta \bar{x}^T \frac{\partial H}{\partial \bar{x}} + \delta \bar{x}^T \frac{\partial \bar{P}}{\partial t} + \Lambda + (-1)^{K-1} \sum_{j=1}^{K} \left( \frac{\partial H}{\partial \bar{x}^j} \right) \left[ \delta \bar{x} \frac{\partial H}{\partial \bar{x}^j} \right] \left( \frac{\partial H}{\partial \bar{x}^j} \right)
\]

\[
+ (-1)^{K} \left[ \delta \bar{x}^T \frac{\partial K}{\partial \bar{x}^K} \frac{\partial H}{\partial (\delta \bar{x}^K)} \right] \, d\Omega dt \quad (2-22)
\]

To obtain the necessary conditions Equation (2-22) is factored and the first variation, \( \delta J \), is set equal to zero. From (2*22)

\[
\delta J = \int_{\Omega} \delta \bar{x}(t_f, \bar{z}) \left[ \frac{\partial \theta_f}{\partial \bar{x}} - \bar{P}(t_f, \bar{z}) \right] \, d\Omega + \int_{t_o}^{t_f} \int_{\Omega} \delta \bar{x}^T \left[ \frac{\partial H}{\partial \bar{x}} + \frac{\partial \bar{P}}{\partial t} \right]
\]
\[ + (-1)^K \left[ \frac{\partial^K}{\partial Z^K} - \frac{\partial H}{\partial \frac{\partial X}{\partial Z^K}} \right] \right\} dt + \int_{t_0}^t \int_{\Omega} \delta u^T \frac{\partial H}{\partial u} dt \]

\[ + \int_{t_0}^t \int_{\Omega} \left\{ \Lambda + (-1)^{K-1} \left( \frac{\partial}{\partial Z} \right)^T \left[ \delta X \frac{\partial^{K-1}}{\partial Z^{K-1}} \frac{\partial H}{\partial \frac{\partial X}{\partial Z^{K-1}}} \right] \right\} dt = 0 \quad (2-23) \]

Integration of the last integral in (2-23) over the spatial coordinates results in

\[ \int_{t_0}^t \int_{\Omega} \left\{ \Lambda + (-1)^{K-1} \left( \frac{\partial}{\partial Z} \right)^T \left[ \delta X \frac{\partial^{K-1}}{\partial Z^{K-1}} \frac{\partial H}{\partial \frac{\partial X}{\partial Z^{K-1}}} \right] \right\} dt = \]

\[ \left. \int_{t_0}^t \left[ \frac{\partial^{K-1}}{\partial Z^{K-1}} \frac{\partial H}{\partial \frac{\partial X}{\partial Z^{K-1}}} - \frac{\partial^{K-2}}{\partial Z^{K-2}} \frac{\partial H}{\partial \frac{\partial X}{\partial Z^{K-2}}} \right] \right|\Omega dt \]

\[ + \int_{t_0}^t (-1)^{K-1} \left( \delta X \right) \frac{\partial^{K-1}}{\partial Z^{K-1}} \frac{\partial H}{\partial \frac{\partial X}{\partial Z^{K-1}}} \right|\Omega dt \quad (2-24) \]

Since the boundary conditions are specified, the first variation, \( \delta \tilde{X} \), at the boundaries is zero. This causes the first integral on the right hand side of (2-24) to be zero. Then, Equation (2-23) is modified to

\[ \delta J = \int_{\Omega} \delta \tilde{X}(t_f, \tilde{Z}) \left[ \frac{\partial f}{\partial \tilde{X}} - \tilde{p}(t_f, \tilde{Z}) \right] d\Omega + \int_{t_0}^t \int_{\Omega} \delta \tilde{X}^T \left\{ \frac{\partial H}{\partial \tilde{X}} + \frac{\partial \tilde{p}}{\partial t} \right\} dt \]
For the first variation, $\delta J$, to be zero for any $\delta x$ and $\delta u$, the coefficients of $\delta x$ and $\delta u$ in Equation (2-25) must be identically zero. Setting the coefficients of $\delta x$ and $\delta u$ in (2-25) gives the necessary conditions for optimality

$$\frac{\partial \theta}{\partial x}(t, z) = 0, \quad t = t_f$$

(2-26)

which is one of the transversality conditions, and

$$\frac{\partial H}{\partial x(t, z)} + \frac{\partial \bar{p}(t, z)}{\partial t} + (-1)^K \left[ \frac{\partial^K}{\partial z^K} \frac{\partial H}{\partial (\frac{\partial x}{\partial z}(t, z))} \right] = 0$$

(2-27)

which is the adjoint or the co-state equation, and

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

(2-28)

which gives the optimal control when there is no constraint on $\bar{u}$. Since $\bar{u} \in \omega$, the Hamiltonian is made as large as possible for the choice of $\bar{u}$, which does not violate the constraints on $\bar{u}$, or

$$H(t, \bar{z}, \bar{x}, \frac{\partial x}{\partial z}, \bar{u}) = \sup_{\bar{u} \in \omega} H(t, \bar{z}, \bar{x}, \frac{\partial x}{\partial z}, \bar{u})$$

(2-29)
The other transversality condition is

\[
\frac{\partial^{K-1}}{\partial z^{K-1}} \frac{\partial H}{\partial z^K} = 0 \quad \Omega = \partial \Omega, \quad t = t_f \quad (2-30)
\]

The problem has been reduced to one of finding the optimal control of system of Equations (2-1) subject to initial condition (2-2), boundary condition (2-3), and constraint Equations (2-4), with cost function (2-5).

The optimal control is obtained by the simultaneous solution of systems of Equations (2-1), (2-27), and (2-28), with the initial and boundary conditions (2-2), (2-3), and (2-30). These are systems of two point boundary value, partial differential equations in the time and the spatial domains.

C. Special Cases

There are few special cases of interest, for which the developed theory in the previous section must be modified:

1. Linear System

For a linear DPS the developed conditions not only are necessary, but they are also sufficient.

2. Space Independent Control

When the admissible control is a function of time only, a new Hamiltonian function \( \tilde{H} \) is defined:

\[
\tilde{H} \triangleq \int_{\Omega} H(t, z, \bar{x}, \frac{\partial x}{\partial z^K}, U(t)) d\Omega \quad (2-31)
\]
Then the optimal \( U^*(t) \) is control which maximizes \( \bar{H} \) for any \( t \in \tau \) and \( U^*(t) \in \omega \).

3. Time Independent Control

When the admissible control is a function of the spatial coordinates only a new Hamiltonian function \( \bar{H} \) is defined:

\[
\bar{H} \triangleq \int_{t_0}^{t_f} H(t, \tilde{Z}, \tilde{X}, \frac{\partial \tilde{X}}{\partial \tilde{Z}}, U(\tilde{Z})) dt
\]

Then the optimal \( U^*(\tilde{Z}) \) is a control which maximizes \( \bar{H} \) for all \( \tilde{Z} \in \Omega \) and \( U(\tilde{Z}) \in \omega \).

In the next chapter the theory just developed and special case 2 will be applied to the optimal control of an actual system. The system is a plug-flow tubular reactor with a consecutive first-order chemical reaction taking place.
CHAPTER III
FEEDFORWARD CONTROL

A. Introduction

As was mentioned in the previous chapter, the developed theories for the optimal control of DPS have not been applied to many practical systems. Most of the early work was devoted to the development of the theory, its application to systems of linear partial differential equations (PDE), and systems with known analytic solutions. Heat transfer to a slab was considered extensively.

Denn (21) used gradient technique to obtain the optimal control of a non-linear PDE with boundary control. Yeh and Tou (82) applied Butkovskii's maximum principle for DPS to a drying process. Briggs and Shen (8) considered minimum-time control of a nuclear rocket described by a DPS subject to thermal stress constraints. The optimal control was obtained by controlling the flow rate of the nuclear fuel. Alvaradro and Muknudan (2) discussed the optimal control of a furnace heating a one-dimensional slab with a quadratic performance index.

The steady state optimal control of tubular reactors, which involves the solution of ordinary differential equations, has been considered by many investigators. But, relatively little is known about the optimal control of unsteady state tubular reactors, which are described by PDE.

Chang and Bankoff (18) investigated the optimal unsteady control of a jacketed tubular reactor for a first-order consecutive reactions subject to step change in the feed concentration. Paradis and
Perlmutter (53) considered the transient behavior of a tubular reactor model in detail. Optimization of a periodic process, involving a tubular reactor with a second-order homogenous reaction, was discussed by Fjeld and Kristiansen (25).

The purpose of this chapter is the application of the theory developed in Chapter II to a particular system. The optimal feedforward control of a tubular reactor with a first order consecutive reactions $A \xrightarrow{K_1} B \xrightarrow{K_2} C$ will be considered.

B. Description of the System

The system consists of a jacketed tubular reactor in which an exothermic, first-order consecutive reaction

$$A \xrightarrow{K_1} B \xrightarrow{K_2} C$$

is taking place. The reactor is of length $L$ (units of length) and its diameter is $r$ (units of length). The generated heat of reaction is removed by flow of cooling water. The reactants $A$ and $B$, with concentration $CA_0$ and $CBO$ g-moles/liter respectively, and temperature $T_0^\circ K$ are fed to the reactor with velocity $v$ (unit of length/minute). The feed is subject to stepwise disturbance. The amount of heat removed from the system is controlled by the temperature of the cooling water $TC(t)$.

It is required to obtain the optimal $TC(t)$ for a given disturbance in the feed composition, such that the cumulative exit concentration of the desired product $B$, $CB$, is maximized during a given period of time $t_f$ (minutes).
The following assumptions have been made in development of a mathematical model for the system:

(a) Constant physical properties for the reactants throughout the length of reactor.

(b) The flow of the reacting fluid is plug-flow; constant velocity throughout the reactor has been assumed.

(c) Axial diffusion is negligible.

(d) There are no radial temperature and concentration gradients.

(e) The heat capacitance of the reactor wall is negligible.

(f) The flow rate of the cooling water is sufficiently large; such that, there is no axial shell-side temperature gradient.

The dynamics of the system are described by a system of partial differential equations (Appendix A):

\[
\begin{align*}
\frac{\partial C_A}{\partial t} &= -K_1 C_A - v \frac{\partial C_A}{\partial z} \\
\frac{\partial C_B}{\partial t} &= K_1 C_A - K_2 C_B - v \frac{C_B}{z} \\
\frac{\partial T}{\partial t} &= b_1 K_1 C_A + b_2 K_2 C_B + \alpha(T_C(t) - T) - v \frac{\partial T}{\partial z}
\end{align*}
\]

(3-1)

Where \(K_1\) and \(K_2\) are the reaction rate constants which are defined by the Arrhenius equation

\[
K_1 = K_{10} \exp\left(-\frac{E_1}{RT}\right) \quad (3-2)
\]

\[
K_2 = K_{20} \exp\left(-\frac{E_2}{RT}\right)
\]

Where \(K_{10}\) and \(K_{20}\) are the frequency factors and \(E_1\) and \(E_2\) are the activation energy; \(T(t,z)\) and \(v\) are the temperature and the velocity of the reactant fluid; \(b_1 = \left(-\frac{\Delta H_A}{C_p \rho}\right)\) and \(b_2 = \left(-\frac{\Delta H_B}{C_p \rho}\right)\) where \(-\Delta H_A\) and
(-ΔH_B) are the heat of reaction per gram mole of A and B respectively, and C_p and \( \rho \) are heat capacity and density of the reacting fluid; and \( \alpha = \frac{2u}{r \cdot C_p \cdot \rho} \), a heat exchange parameter, where \( u \) is the overall heat transfer coefficient and \( r \) is the tube radius.

The initial conditions of the system are given by the concentration and the temperature of the feed:

\[
\begin{align*}
CA(t,0) &= CA_0 \\
CB(t,0) &= CB_0, \quad 0 < t \leq t_f, \quad z = 0 \\
T(t,0) &= T_0
\end{align*}
\]

(3-3)

The boundary conditions are given by

\[
\begin{align*}
CA(0,z) &= d_A(z) \\
CB(0,z) &= d_B(z), \quad 0 \leq z \leq L, \quad t = 0 \\
T(0,z) &= d_T(z)
\end{align*}
\]

(3-4)

which are obtained by solving the steady state equations of the system.

The cost function, which must be minimized, is defined as

\[
J = -\int_0^{t_f} CB(t,L)dt = -\int_0^{t_f} \int_0^L \frac{\partial CB(t,z)}{\partial z} dzdt
\]

(3-5)

C. Formulation of Open Loop Optimal Control

The Hamiltonian for the system is formed according to Equation (2-9):

\[
H = \frac{\partial CB}{\partial z} + P_1 \left( -K_1CA - \frac{\partial CA}{\partial z} \right) + P_2 \left( K_1CA - K_2CB - \frac{\partial CB}{\partial z} \right) + P_3 \left( b_1K_1CA + b_2K_2CB + \alpha(T_C(t) - T) - \frac{\partial T}{\partial z} \right)
\]

(3-6)

where \( P_1, P_2 \) and \( P_3 \) are the adjoint or costate variables. The system
of the adjoint variables are obtained according to Equation (2-27):

\[ \frac{\partial P_1}{\partial t} = K_1 P_1 - K_2 P_2 - b_1 K_1 P_3 - v \frac{\partial P_1}{\partial z} \]

\[ \frac{\partial P_2}{\partial t} = K_2 P_2 - b_2 K_2 P_3 - v \frac{\partial P_2}{\partial z} \quad (3-7) \]

\[ \frac{\partial P_3}{\partial t} = \frac{E_1}{RT^2} K_1 C A P_1 - \frac{1}{RT^2} (E_1 K_1 C A - E_2 K_2 C B) P_2 \]

\[ - \frac{1}{RT^2} (b_1 E_1 K_1 C A + b_2 E_2 K_2 C B) P_3 + \alpha P_3 - v \frac{\partial P_3}{\partial z} \]

The final conditions on the adjoint variables are defined by Equation (2-26)

\[ P_i(t,z) = 0, \quad i = 1,3, \quad t = t_f \quad \text{and} \quad 0 \leq z \leq L \quad (3-8) \]

The boundary conditions on the adjoint variables are obtained by using the transversality condition Equation (2-30).

\[ \frac{\partial H}{\partial z} = - v P_1 = 0 \]

\[ \frac{\partial H}{\partial z} = + 1 - v P_2 = 0, \quad t = t_f, \quad z = 0 \quad (3-9) \]

\[ \frac{\partial H}{\partial z} = - v P_3 = 0 \]

or

\[ P_1(t_f,0) = 0 \]

\[ P_2(t_f,0) = + \frac{1}{v} \quad (3-10) \]

\[ P_3(t_f,0) = 0 \]

To obtain the optimal control; Equation (3-1) subject to the initial and boundary conditions of Equations (3-3) and (3-4) are solved
forward in time. Equation (3-7), subject to the initial and the boundary conditions of (3-9) and (3-10), are solved backward in time. Thus, the Hamiltonian (Equation 3-6) is maximized with respect to the choice of TC. The solution considers a system of two-point boundary-value, six partial differential equations simultaneously.

D. Gradient Technique

The mathematics of the gradient technique, or the method of steepest descent, was originally formulated by Cauchy (1860). The method was introduced in the computational solution of the optimal control theory by Kelley (33) and also independently by Bryson and Denham (10).

The gradient technique basically is an iterative procedure which satisfies the system and the constraint equations and improves the objective or cost function with each iteration. The main advantage of the gradient method is the relative independence of the convergence on the initial guess of the optimal control vector. The greatest disadvantage of the method is the slow iteration convergence in the neighborhood of the optimum.

In this section the method is developed for the system Equation (2-1) and then applied to the particular system of interest. It is required to minimize the cost function (2-5) subject to a system of Equations (2-1), initial condition (2-2) and boundary condition (2-3). Mathematically the solution is obtained by solving the state equations forward in time and the adjoint equations backwards in time using the control relation (2-28) and the given initial and boundary conditions on the state and the adjoint variables. However, the solution to Equation (2-28), if not formidable, is not easy.
The general procedure in using the gradient technique is to first assume a solution for the control vector \( \tilde{U}(t, \tilde{z}) \) in the first iteration. Since the assumed control is not the optimal control, the relation \( \frac{\partial H}{\partial \tilde{U}} = 0 \) does not hold. For this initial control, the trajectory, the adjoint variables, and the cost function are calculated from their respective equations. In the subsequent iteration, a new control vector is chosen which is different from the initial control, \( \tilde{U}(t, \tilde{z}) \), by an amount \( \Delta \tilde{U}(t, \tilde{z}) \). The cost function together with the trajectory and the adjoint variables are evaluated for this new control vector. The change in the cost function is obtained from (2-24).

\[
\Delta J = \int_{t_0}^{t_f} \int_{\Omega} \left( \frac{\partial H}{\partial \tilde{U}} \right)^T \Delta \tilde{U}(t, \tilde{z}) d\Omega dt
\]  

(3-11)

If the largest change in \( \Delta J \), in the decreasing direction of \( J \), is desired, the distributed control should be in the direction of the gradient of the Hamiltonian computed from the present trajectory and adjoint solution:

\[
\Delta U_j(t, \tilde{z}) = + \varepsilon \frac{\partial H}{\partial U_j} \quad J = 1, \ldots, M
\]  

(3-12)

where \( \varepsilon \) is the step size of iteration.

Now applying the developed gradient technique to the system, a control vector \( \tilde{U}(t, \tilde{z}) \), is assumed. The state variables \( \tilde{x}^o(t, \tilde{z}) \) are calculated, from the system equations and their initial and boundary conditions for all \( t \in [t_0, t_f] \). Then, by the backward integration of the system of the adjoint equations, using the terminal and the boundary conditions on the adjoint variables, \( \tilde{P}(t, \tilde{z}) \) are obtained for all \( t \in [t_f, t_0] \).
Then the gradient of the Hamiltonian, \( \frac{\partial H}{\partial \tilde{U}} \), is calculated from

\[
\frac{\partial H}{\partial \tilde{U}} = \frac{\partial \varphi}{\partial \tilde{U}} + \frac{\partial f}{\partial \tilde{U}} \tilde{P}, \quad \tilde{X} = \tilde{X}^o(t,z), \quad \tilde{P} = \tilde{P}^o(t,z), \quad \tilde{U} = \tilde{U}^o(t,z)
\] (3-13)

and \( \Delta \tilde{U}^o \) is determined from Equation (2-17). A new trial value of \( \tilde{U} \) is given by:

\[
\tilde{U}'(t,z) = \tilde{U}^o(t,z) + \Delta \tilde{U}^o(t,z)
\] (3-14)

The procedure is repeated until the change in the control vector or the cost function is negligible from one iteration to the next.

If the control vector \( \tilde{U} \) is not a function of \( z \), then Equation (3-12) becomes

\[
\Delta \tilde{U}(t) = \tilde{\epsilon}_p \int_\Omega \left( \frac{\partial H}{\partial \tilde{U}} \right) \, d\Omega
\] (3-12a)

and if it is not a function of \( t \), then Equation (3-12) becomes

\[
\Delta \tilde{U}(t) = \tilde{\epsilon}_p \int_t^f \left( \frac{\partial H}{\partial \tilde{U}} \right) \, dt
\] (3-12b)

The step size \( \tilde{\epsilon}_p \) should be small enough to insure the condition \( \Delta J < 0 \), but on the other hand, should be large to assure fast convergence. The iterations are terminated whenever the improvement in the absolute value of the cost function is less than a small positive number, \( \tilde{\epsilon}_S \). Usually, at the initial iteration, \( \tilde{\epsilon}_p \) is small and it is made larger at the end of each successful iteration. A successful iteration is one which decreases the cost function.

E. Computational Scheme

After choosing a control vector, \( \tilde{U}(t) \), the system and the adjoint equations must be solved. The solution involves solving six partial differential equations (PDE). There is also the problem of the split
boundary conditions.

To obtain the solution, the PDE must be discretized. Discretization is accomplished by one of the following forms:

1) Spatial discretization. This scheme involves the replacement of the spatial partial derivatives by their approximately equivalent difference equations. The result would be a system of ordinary differential equations in time.

2) Time discretization. The partial derivatives with respect to the time are replaced by their approximately equivalent difference equations. A system of ordinary differential equations in the spatial domain are obtained.

3) Space-time discretization. In this case all the partial derivatives are replaced by their approximately equivalent difference equations; the result is a system of difference equations.

Chang and Bankoff (18) have solved this problem, using the method of characteristics for partial differential equations. Wismir (80) considered a parabolic PDE. By using the spatial discretization technique the PDE was replaced by a larger set of ordinary differential equations. The set of the ordinary differential equations were decomposed into several independent subsets of the lower dimensions. Then, each subset was treated separately and the results were combined to obtain the overall optimal control. It is also possible to use the same technique for time-discretization.

The technique which is used here is based on spatial-time discretization. For the purpose of this problem, the spatial coordinate, z, varies between 0 and 1; and the time variable, t, increases
from zero to the final time $t_f$. Thus, the portion of the $\Omega$ described is the strip in the positive half-plane among the lines $z = 0$, $z = 1$, $t = 0$, and $t = t_f$. This is the area shown in Figure 3-1.

The independent variables are replaced by discrete variables which are defined at points located as shown in the Figure 3-1. The region between 0 and 1 along the $z$ axis is divided into $I$ increments of size $\Delta z$, with grid points being located on the boundary.

The time axis is divided into increments of size $\Delta t$. The grid points at which the dependent variables are to be computed are represented by the circles in Figure 3-1.

The index $i$ refers to the position along the spatial coordinate $z$ and the index $n$ denotes the position along the $t$ axis. The value of the discrete variable $z$ at a grid point is given by

$$z_i = i(\Delta z)$$
The values of the discrete time are obtained from

\[ t_n = n(\Delta t) \]

Each dependent variable is a function of the two discrete independent variables, \( z_i \) and \( t_n \). Therefore, two subscripts are needed to show a dependent variable at a point; thus

\[ \tilde{x}(t_i, z_n) \equiv \tilde{x}(i, n) \]

The initial conditions are given for \( n = 0 \); and the boundary conditions are specified at \( i = 0 \). Each row of the points in Figure 3-1 is referred to as a time level. The values of the dependent variables at the zero\(^{th}\) time level are given by the boundary conditions.

By using the values of the dependent variables at the zero\(^{th}\) level, the values of the variables in the first time level, \( n = 1 \), are found. The process is continued by obtaining the values of the dependent variables at each time level by the use of the known values of the dependent variables in the previous time level. It is assumed that the values of the dependent variables in the time level \( n \) are known, while the values of the dependent variables in the time level \( n+1 \) are to be calculated.

To obtain the solution to the system equations, the time and spatial derivatives must be replaced by their equivalent finite difference equations.

A centered difference analog was used in which the derivatives were centered in both time and space with respect to the grid points. A sample point is designated by \((\star)\) and is shown in Figure 3-1. The coordinates of this point are \((i - \frac{1}{2}, n + \frac{1}{2})\).
Using the method of von Rosenberg (72) in solving partial differential equations, the time derivatives are approximated as

\[
\left( \frac{\partial \tilde{X}}{\partial t} \right)_{i+\frac{1}{2}, n+\frac{1}{2}} \approx \frac{1}{2} \left( \frac{\tilde{X}_{i+1, n+1} - \tilde{X}_{i, n}}{\Delta t} + \frac{\tilde{X}_{i-1, n+1} - \tilde{X}_{i-1, n}}{\Delta t} \right) \quad (3-15)
\]

The spatial derivatives are replaced by

\[
\left( \frac{\partial \tilde{X}}{\partial z} \right)_{i+\frac{1}{2}, n+\frac{1}{2}} \approx \frac{1}{2} \left( \frac{\tilde{X}_{i+1, n+1} - \tilde{X}_{i-1, n+1}}{\Delta z} + \frac{\tilde{X}_{i, n} - \tilde{X}_{i-1, n}}{\Delta z} \right) \quad (3-16)
\]

The values of the dependent variables at the point \((i+\frac{1}{2}, n+\frac{1}{2})\) are approximated by

\[
\tilde{X}_{i+\frac{1}{2}, n+\frac{1}{2}} \approx \frac{1}{4} \left( \tilde{X}_{i+1, n+1} + \tilde{X}_{i, n} + \tilde{X}_{i-1, n+1} + \tilde{X}_{i-1, n} \right) \quad (3-17)
\]

These equations are substituted in the system equations with the appropriate initial and boundary conditions. After some algebraic manipulation, a system of equations is obtained which allows one to calculate the values of the dependent variables at the time level \(n+1\) in terms of the variables at the time level \(n\). This process is continued until the final time, \(t_f\), has been reached.

Since, in this case the system of equations has a dependent variable in the argument of an exponential, it is not possible to solve explicitly for the unknown dependent variables at the time level \(n+1\). To remove this difficulty an iterative procedure was devised. In the first iteration it is assumed that the unknown variables at the time level \(n+1\) have the same values as at time level \(n\); therefore, Equation (3-17) is reduced to

\[
\tilde{X}_{i+\frac{1}{2}, n+\frac{1}{2}} \approx \frac{1}{2} \left( \tilde{X}_{i-1, n} + \tilde{X}_{i, n} \right) \quad (3-18)
\]
Substitution of Equation (3-18) results in a system of equations which gives the values of the unknown variables at the time level \( n+1 \). These values are now substituted into Equation (3-17) and the result is used in the system equations to recalculate the values of the dependent variables at the time level \( n+1 \). This process is repeated until there is not significant difference in the value of each dependent variable.

In order to obtain the optimal control to step disturbance in feed, the following procedure is used:

1) An initial control, \( TC^0(t) \), is assumed.

2) The \( z \) axis is divided in \( I \) equal segments of length \( \Delta z \); and the \( t \) axis is divided in equal segments of the length \( \Delta t \).

3) The system equations are discretized in the described manner.

4) The finite difference equivalents for the system of the adjoint equations are obtained.

5) The system's finite difference equations are solved forward in time and the results are stored.

6) The adjoints' finite difference equivalents are integrated backward in time using, the final and boundary conditions on the adjoint variables, and the stored values of the state variables.

7) In order to maximize the Hamiltonian, \( H \), with respect to the choice of the control, \( TC(t) \):

\[
\frac{\partial H}{\partial TC(t)} = \int_0^1 \alpha P_3(t,z) dz \tag{3-19}
\]

is evaluated.

8) A proportionality constant, \( \epsilon_p \), is selected for the iteration.
9) The new value of the control, \( TC'(t) \) for the next iteration, is given by

\[
TC'(t) = TC^0(t) + \epsilon \int_0^1 \alpha \ P_3(t,z) \, dz
\]  

(3-20)

10) The new control, \( TC'(t) \), is used and steps 5 through 10 are repeated; till there is no significant change in the control vector, or improvement in the cumulative yield of \( B \).

F. Steady State Solution

In order to obtain the initial conditions on the state variables, Equation (3-4), the steady state solution of the system equations, Equation (3-1), must be found. This is accomplished by setting the partial derivatives with respect to time equal to zero. This reduces the system's equations to

\[
\frac{dCA}{dz} = -\frac{K_1}{v} CA
\]

\[
\frac{dCB}{dz} = \frac{K_1}{v} CA - \frac{K_2}{v} CA
\]

\[
\frac{dT}{dz} = \frac{b_1 K_1}{v} CA + \frac{b_2 K_2}{v} CB + \alpha (TC(t) - T)
\]

(3-21)

The initial conditions for the system of equations (3-21) are specified by Equation (3-3).

For the purpose of the numerical solution, the following values for the parameters were taken from Bilous and Amundson (6):

\[
K_{10} = 5.35 \times 10^{10} \text{ min}^{-1}
\]

\[
K_{20} = 4.61 \times 10^{17} \text{ min}^{-1}
\]
\[ E_1 = 18,000 \text{ cal/mole} \]
\[ E_2 = 30,000 \text{ cal/mole} \]
\[ R = 2 \text{ g-cal/(g-mole)(°K)} \]

In addition, it was assumed the reaction generated heat, the following values for the additional parameters were selected from Chang and Bankoff (18):

\[ \alpha = 1/3 \text{ min}^{-1} \]
\[ L = 1 \text{ unit of length} \]
\[ v = 0.1 \text{ unit of length/minute} \]
\[ b_1 = 100 \text{ Lit - °K/g-mole} \]
\[ b_2 = -50 \text{ Lit - °K/g-mole} \]

The value of \( v \) corresponds to setting the residence time equal to ten minutes.

Initially the reactor is assumed to be at steady state with the following feed concentration and temperature

\[ \text{CAO} = 0.95 \text{ g-mole/liter} \]
\[ \text{CBO} = 0.05 \text{ g-mole/liter} \]
\[ \text{TO} = 331.4 \text{ °K} \]

At time \( t = 0 \), the feed is subject to a step disturbance which results in the following changes

\[ \text{CAO} = 0.65 \text{ g-mole/liter} \]
\[ \text{CBO} = 0.35 \text{ g-mole/liter} \]
\[ \text{TO} = 300 \text{ °K} \]

The Pattern Search Technique (79) was used to obtain the optimal steady state value of the control, \( TC(t) \), the results are tabulated in Table 1.
TABLE 1. STEADY STATES

<table>
<thead>
<tr>
<th></th>
<th>CA0</th>
<th>CBO</th>
<th>TO</th>
<th>TC(t)</th>
<th>CB(1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>0.95</td>
<td>0.05</td>
<td>331.4</td>
<td>316.4</td>
<td>0.66276</td>
</tr>
<tr>
<td>New</td>
<td>0.65</td>
<td>0.35</td>
<td>300.0</td>
<td>331.7</td>
<td>0.66577</td>
</tr>
</tbody>
</table>

The optimal values of the control, Tc(t), were substituted in Equation (3-21). The reactor length was divided into 20 equal segments with Δz = 0.05 units of length. The fourth-order Runge-Kutta method was used to integrate the equations to obtain the initial profiles. The initial concentrations and temperature profiles are plotted in Figures 3-2 and 3-3, respectively; these are the required boundary conditions given by Equation (3-4).

The new steady state profiles of concentrations and temperature are shown by Figures 3-4 and 3-5. If there is no further disturbance in the feed, after sufficient time, the transient concentrations and temperature profiles would approach the new steady state solution. The steady state temperature profiles show initially that cooling water cools the entire length of the reactor, but after the step disturbance in the feed only the rear half of the reactor is being cooled.

G. Synthesis of Optimal Control

Assume the jacketed tubular reactor has been in operation, at the optimal steady state, up to the time t = 0⁻. At the time t = 0⁺, the feed condition from CA = 0.95, CB = 0.05, and T = 331.4°K is
OPTIMAL STEADY STATE SOLUTION CONCENTRATION PROFILE

LEGEND

<table>
<thead>
<tr>
<th>CA(Z)</th>
<th>CB(Z)</th>
</tr>
</thead>
</table>

FIGURE 3-2

CONCENTRATION G-MOLE/LITER

REACTOR LENGTH
OPTIMAL STEADY STATE SOLUTION TEMPERATURE AND CONTROL PROFILE

Legend

T(Z)  

TC

FIGURE 3-3
NEW OPTIMAL STEADY STATE SOLUTION AFTER STEP DISTURBANCE IN FEED
CONCENTRATION PROFILE

LEGEND

<table>
<thead>
<tr>
<th>CA(Z)</th>
<th>CB(Z)</th>
</tr>
</thead>
</table>

FIGURE 3-4

CONCENTRATION (G-MOLE/LITER)

REACTOR LENGTH
NEW OPTIMAL STEADY STATE SOLUTION AFTER STEP DISTURBANCE IN FEED TEMPERATURE AND CONTROL PROFILE

LEGEND


\( T(z) \)

\( T_c \)

FIGURE 3-5
suddenly subject to a step change with $CA = 0.65$, $CB = 0.35$, and $T = 300^\circ K$. It is required to find a control, $T_C(t)$, which maximizes the cumulative yield of $B$ during a time interval $[0,25]$ minutes.

As it was described in the previous section, the steady state optimal values of the control $T_C(t)$ were obtained using the Pattern Search Technique. It is possible to use the steady state values of the control $T_C(t)$. If the old steady state value of $T_C(t)$ is used, there would not be any control action on the step disturbance in the feed conditions. The result of the application of this control is given in Figure 3-6. The instantaneous yield of $B$, which is the exit concentration of $B$, remains constant for one residence time after the initial disturbance. Then, there is a sharp discontinuity at $t = 10$ minutes. After the sharp discontinuity, the exit concentration of $B$ remains constant at its new steady state value. The cumulative yield of $B$ for this case was 13.233 g-mole/liter.

The results of the application of the new optimal steady state value of $T_C(t)$ is given in Figure 3-7 and is compared with the results of using the old steady state value of $T_C(t)$. In this case the exit concentration of $B$ starts to change immediately after the step change in the feed conditions. The exit concentration of $B$ reaches the new steady state in about 12.5 minutes. The discontinuity in the instantaneous yield is still present around one residence time. The cumulative yield in this case is 15.346 g-mole/liter which is higher than the yield using no control action. The higher yield is mainly due to the higher steady state value of the exit concentration of $B$ using new optimal steady state concentration.
STABLE STATE CONTROL TO STEP DISTURBANCE IN FEED INSTANTANEOUS YIELD WITH NO CONTROL

LEGEND

FIGURE 3-6
STEADY STATE CONTROL TO STEP DISTURBANCE IN FEED
INSTANTANEOUS YIELD WITH NEW STEADY STATE OPTIMAL CONTROL

LEGEND

- OLD STEADY STATE CONTROL  - NEW STEADY STATE CONTROL

FIGURE 3-7
The optimal control was obtained by making an initial guess of $\text{TC}(t) = 331.7^\circ K$ for $t \in [0, 25]$. Since the time axis was divided into a finite number of grid points, the values of $\text{TC}(t)$ were assigned at these points.

For the first iteration the initial guess of the control was used to solve the system equations. The values of $\text{CA}$, $\text{CB}$, and $T$ at each grid point were stored for the backward integration of the adjoint equations. After the adjoint variables for the entire grid points were obtained, the integration $\int_0^1 P \, dz$ was evaluated by Simpson's one-third rule. A proportionality constant, $\epsilon_p$, was selected and the value of the integral was multiplied by this constant. Using Equation (3-14) at each time-step an improved control was calculated. The new control was applied to the system and the cumulative yield was calculated. If the new cumulative yield was less than the previous one, the proportionality constant was decreased and using Equation (3-14) a new control was obtained. This process was repeated until a higher new yield was obtained. After the proper proportionality constant was obtained, the calculations progressed to the next iteration. The iterations were stopped whenever the improvement in the yield from one iteration to the next was less than a chosen constant, $\epsilon_s$.

The optimal control, $\text{TC}(t)$ and the corresponding optimal yield are plotted in Figures 3-8 and 3-9. At $t = 0^+$, the optimal control $\text{TC}(t)$ drops to a value lower than the steady state value, then, in a zigzag pattern increases to a peak. It then settles down with a damped oscillation to the new steady state optimal control, but
Figure 3A8
OPTIMAL YIELD AFTER STEP DISTURBANCE
EXIT CONCENTRATION OF B

LEGEND

FIGURE 3-9
there is a sharp rise one residence time before the final time is reached. The sharp rise is explained by reasoning that the control within one residence time from the final time does not have to be optimal for the portion of the reactant fluid still in the reactor at the final time. The optimal instantaneous yield, Figure 3-9, shows a discontinuity around one residence time after the initial disturbance. This is a result of initial discontinuity in the feed conditions at \( t = 0 \), which propagates throughout the reactor.

The effects of the new steady state control and the optimal control on the yield are compared in Figure 3-10. The optimal yield is 16.1805 g-mole/liter; the yield using the new steady state control is 15.343 g-mole/liter which is less than the optimal yield. The new and the old steady state controls were compared in the Figure 3-7. The yield using the old steady state control (no control action to the disturbance) is 13.233 g-mole/liter which is considerably less than the optimal control.

The convergence of the iterations were dependent on the initial guess of the control, \( T_C(t) \); the proportionality constant for the iterations, \( \epsilon_p \); and the change in the proportionality constant, \( \Delta \epsilon_p \), from one iteration to the next. Three different initial guesses of the control were made. The resulting optimal controls are plotted in Figures 3-11, 3-12, and 3-13. It is observed that in each case the same optimal control was obtained. In every case, rapid convergence is observed by the tenth iteration, but a small \( \epsilon_s \) needs more iterations.

A search was done to obtain the optimal value of \( \epsilon_p \) and \( \Delta \epsilon_p \).
OPTIMAL YIELD AFTER STEP DISTURBANCE
NEW STEADY STATE CONTROL VS. OPTIMAL CONTROL

FIGURE 3-10
CONVERGENCE WITH RESPECT TO INITIAL CONTROL
INITIAL CONTROL TC(T) = 331.7

LEGEND

⊙ INITIAL GUESS
△ ITERATION NO. 5
◆ ITERATION NO. 10
▲ ITERATION NO. 15
★ ITERATION NO. 20
♦ OPTIMAL CONTROL

![Graph showing convergence with respect to initial control](image)

FIGURE 3-11
CONVERGENCE WITH RESPECT TO INITIAL CONTROL

INITIAL CONTROL $TC(T) = 316.4 + 0.306 \times T$

<table>
<thead>
<tr>
<th>Legend</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>□</td>
<td>INITIAL GUESS</td>
</tr>
<tr>
<td>▲</td>
<td>ITERATION NO. 10</td>
</tr>
<tr>
<td>□</td>
<td>ITERATION NO. 15</td>
</tr>
<tr>
<td>□</td>
<td>ITERATION NO. 20</td>
</tr>
<tr>
<td>□</td>
<td>OPTIMAL CONTROL</td>
</tr>
</tbody>
</table>

**Figure 3-12**

TIME (MIN.)
CONVERGENCE WITH RESPECT TO INITIAL CONTROL

LEGEND

- INITIAL GUESS
- ITERATION NO. 5
- ITERATION NO. 10
- OPTIMAL CONTROL

FIGURE 3-13
The smaller the value of the proportionality constant, $\epsilon_p$, the slower the convergence of the iterations. High values of $\epsilon_p$ caused instability of the solution. A compromise was made between the stability of the solution and rapid convergence; and $\epsilon_p = 200$, for the first iteration, was selected. Using this value of $\epsilon_p$, the effect of $\Delta \epsilon_p$ was observed on the convergence. The results are tabulated in Table 3-2.

**TABLE 2. EFFECT OF $\Delta \epsilon_p$ ON CONVERGENCE OF ITERATIONS**

<table>
<thead>
<tr>
<th>$\epsilon_p$</th>
<th>$\Delta \epsilon_p$</th>
<th>Iteration No.</th>
<th>Yield $\text{g-mole liter}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>10</td>
<td>18</td>
<td>16.176</td>
</tr>
<tr>
<td>200</td>
<td>20</td>
<td>17</td>
<td>16.178</td>
</tr>
<tr>
<td>200</td>
<td>25</td>
<td>14</td>
<td>16.175</td>
</tr>
<tr>
<td>200</td>
<td>30</td>
<td>12</td>
<td>16.172</td>
</tr>
</tbody>
</table>

Even though the high value of $\Delta \epsilon_p$ seems to be desirable, using $\Delta \epsilon_p = 30$ violated the requirement for the positive change in the cost function near the optimum. There were also some problems associated with stability near the optimum solution. The best value of $\Delta \epsilon_p$ was found to be 20, and this value was used to obtain the optimal solution.
A. Introduction

In this chapter the approximate transfer functions of the reactor system will be developed. It is then possible to approximate the system's dynamics and to design an optimal feedforward control. The approximate transfer function makes it possible to reduce the distributed parameter system to a lumped parameter system and thereby apply the more simplified optimal control theory for these type systems.

In order to obtain the approximate transfer function it is desirable to obtain the corresponding frequency response. This may be accomplished by forcing of the system with a sinusoidal input, pulse testing, or using a technique that involves taking the Laplace transform of the partial differential equations. Since the Laplace transform is a linear operator the system of nonlinear partial differential equations must first be linearized about a particular operating point.

Once the frequency response has been obtained a suitable functional form for the transfer functions is selected and fitted to the frequency response. Finally, the obtained transfer functions are inverted into time domain and the resulting time domain response is compared with the actual response to observe the effect of approximations.

The first point to be discussed in this chapter involves the development of linearized partial differential equations. This is
the subject of the following section.

B. **Linearization**

Control theory is far more advanced for linear systems than for non-linear systems. The most attractive features of the linear systems are: the relative ease of mathematical manipulations and calculations of the linear equations; availability of transform techniques; and finally, the validity of the principle of superposition. (The principle of superposition states that the response of a linear system to the combination of two or more input signals is the same as the combinations of the individual responses had each input signal acted upon the system independently).

However most practical chemical processes are non-linear and are therefore not amenable to linear control theory. Therefore, linearization of non-linear system in order to apply linear control theory is frequently done with considerable success.

Linearization may be accomplished by two distinct methods. The first method of linearization is by the variable transformation. In this method the non-linear terms are replaced by newly defined linear variables. Koppel (52) has used this technique to obtain the dynamics and the optimal control of non-linear, distributed-parameter, chemical reactors. The second and more extensively used method of linearization is based on the truncated Taylor series expansions of the non-linear terms about a steady state. This is the method which is used in this work.

The multivariable Taylor series expansion of a function \( F(x,y) \) about a equilibrium state \( (x_e,y_e) \) can be represented by
\[
F(x,y) = F(x_e,y_e) + \left. \frac{\partial F}{\partial x} \right|_{x_e} \Delta x + \left. \frac{\partial F}{\partial y} \right|_{y_e} \Delta y + \text{non-linear terms}
\]  
\hspace{1cm} \text{(4-1)}

where \( \Delta x \) and \( \Delta y \) are the deviations from the equilibrium state defined as

\[
\Delta x = x - x_e, \quad \Delta y = y - y_e
\]  
\hspace{1cm} \text{(4-2)}

and the partial derivatives are evaluated at the equilibrium state. Neglecting the non-linear terms in the Equation (4-1) would result in a linear equation.

Before proceeding to linearize the system's equations, it is desirable to write the equations in dimensionless form. To obtain the dimensionless system's equations the following dimensionless variables are introduced:

\[
\tilde{Z} = \frac{Z}{L}, \quad \tilde{V} = \frac{V}{V_0}, \quad \tilde{t} = \frac{tV_0}{L}
\]
\[
\tilde{C}_A = \frac{C_A}{C_A0}, \quad \tilde{C}_B = \frac{C_B}{C_A0}, \quad \tilde{T} = \frac{T - T_0}{\Delta T}
\]
\[
\tilde{c} = \frac{c}{V_0}, \quad \tilde{C}_C = \frac{T_c - T_0}{\Delta T}
\]
\[
\tilde{K}_{10} = K_{10} \left( \frac{L}{V_0} \right) \exp(-A), \quad \tilde{K}_{20} = K_{20} \left( \frac{L}{V_0} \right) \exp(-B)
\]

where

- \( L \) = The reactor length units of length
- \( V_0 \) = The initial feed flow rate units of length/min.
- \( C_A0 \) = The initial concentration of the reactant A in the feed g-mole/lit.
- \( T_0 \) = The initial feed temperature
\[ \Delta T = b_1 \text{CAO} \, ^\circ K \]
\[ A = E_1/R \, \text{TO} \]
\[ B = E_2/R \, \text{TO} \]

The dimensionless variables are substituted into Equation (2-3), which result in the following dimensionless equations:

\[
\frac{\partial \tilde{C}_A}{\partial \tilde{t}} = -\tilde{K}_{10} \exp\left(\frac{\Delta T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C}_A - \tilde{V} \frac{\partial \tilde{C}_A}{\partial \tilde{Z}} \\
\frac{\partial \tilde{C}_B}{\partial \tilde{t}} = \tilde{K}_{20} \exp\left(\frac{\Delta T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C}_B - \tilde{V} \frac{\partial \tilde{C}_B}{\partial \tilde{Z}}
\]

\[
\frac{\partial \tilde{T}}{\partial \tilde{t}} = \tilde{K}_{10} \exp\left(\frac{\Delta T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C}_A + \left(\frac{b_2}{b_1}\right) \tilde{K}_{20} \exp\left(\frac{BT}{\tilde{T} + \tilde{T}^*}\right) \tilde{C}_B \\
+ \tilde{\alpha} (\tilde{T}_C - \tilde{T}) - \tilde{V} \frac{\partial \tilde{T}}{\partial \tilde{Z}}
\]

where

\( \tilde{t} = \text{dimensionless time} \)
\( \tilde{Z} = \text{dimensionless length} \)
\( \tilde{K}_{10} \text{ and } \tilde{K}_{20} = \text{dimensionless rate constants} \)
\( \tilde{C}_A \text{ and } \tilde{C}_B = \text{dimensionless concentrations} \)
\( \tilde{T} = \text{dimensionless reactor temperature} \)
\( \tilde{T}_C = \text{dimensionless cooling water temperature} \)
\( \tilde{\alpha} = \text{dimensionless heat exchanger parameter} \)
\( \tilde{T}^* = \text{TO}/\Delta T \)

Now, the system of equations above are linearized by writing the truncated Taylor series expansion about the initial steady state.

The result is
\[ \frac{\partial \bar{C}_A}{\partial t} = -\Omega_A \bar{C}_A - \Omega_T \bar{T} - \bar{V} \frac{\partial \bar{C}_A}{\partial z} \]

\[ \frac{\partial \bar{C}_B}{\partial t} = \Omega_A \bar{C}_A + \Omega_T \bar{T} - \Omega_B \bar{C}_B - \Omega_{TB} \bar{T} - \bar{V} \frac{\partial \bar{C}_B}{\partial z} \]  \hspace{1cm} (4-4)

\[ \frac{\partial \bar{T}}{\partial t} = \Omega_A \bar{C}_A + \Omega_T \bar{T} + \left( \frac{b_2}{b_1} \right) \Omega_B \bar{C}_B + \left( \frac{b_2}{b_1} \right) \Omega_{TB} \bar{T} + \alpha(\bar{T}_C - \bar{T}) - \bar{V} \frac{\partial \bar{T}}{\partial z} \]

where

\[ \bar{C}_A = \bar{C}_A - \bar{C}_{A_{ss}} \]

\[ \bar{C}_B = \bar{C}_B - \bar{C}_{B_{ss}} \]

\[ \bar{T} = \bar{T} - \bar{T}_{ss} \]

\[ \bar{T}_C = \bar{T}_C - \bar{T}_{C_{ss}} \]

\[ \Omega_1 = K_{10} \exp\left( \frac{A_T}{T+T'} \right) \bar{C}_A, \quad \Omega_2 = K_{20} \exp\left( \frac{B_T}{T+T'} \right) \bar{C}_B \]

\[ \Omega_A = \left. \frac{\partial \Omega_1}{\partial \bar{C}_A} \right|_{ss} \]

\[ \Omega_B = \left. \frac{\partial \Omega_2}{\partial \bar{C}_B} \right|_{ss} \]

\[ \Omega_T = \left. \frac{\partial \Omega_1}{\partial \bar{T}} \right|_{ss} \]

\[ \Omega_{TB} = \left. \frac{\partial \Omega_2}{\partial \bar{T}} \right|_{ss} \]

All the parameters with the subscript (ss) refer to the steady state value of the parameters. Since it is assumed that the feed flow rate is constant at \( V_0 \), then
\[ \bar{V} = \frac{V}{V_0} = \frac{V_0}{V_0} = 1 \]  

Equation (4-5) is substituted in (4-4) and results in

\[ \frac{\partial \bar{C_A}}{\partial \bar{e}} = -\Omega_A \bar{C_A} - \Omega_T \bar{T} - \frac{\partial \bar{C_A}}{\partial \bar{Z}} \]

\[ \frac{\partial \bar{C_B}}{\partial \bar{e}} = \Omega_A \bar{C_A} + \Omega_T \bar{T} - \Omega_B \bar{C_B} - \Omega_B \bar{T} - \frac{\partial \bar{C_B}}{\partial \bar{Z}} \]  

\[ \frac{\partial \bar{T}}{\partial \bar{e}} = \Omega_A \bar{C_A} + \Omega_T \bar{T} + \frac{b_2}{b_1} \Omega_B \bar{C_B} + \frac{b_2}{b_1} \Omega_B \bar{T} + \bar{a}(\bar{C} - \bar{T}) - \frac{\partial \bar{T}}{\partial \bar{Z}} \]  

The system of Equations (4-6) are the final form of the linearized and the dimensionless system equations which will be used in the subsequent sections.

C. Linear vs Nonlinear Response

As stated above linearization is an approximation. Whenever a system is approximated some of its inherent properties are destroyed. However, a good approximation is one which has most of the inherent properties of the actual system and neglects the less important characteristics of the system. The solution for such an approximate system would be in the neighborhood of the actual solution. Therefore, it is valuable to compare the response of the nonlinear system and the corresponding linear system to a step disturbance in the feed conditions.

The response of the nonlinear system is obtained as discussed in
the previous chapter. To obtain the response of the linear system, the coefficients $\Omega_A$, $\Omega_B$, $\Omega_T$, and $\Omega_{TB}$ must be evaluated. These coefficients are functions of space variable, $\tilde{Z}$, and are called the sensitivity functions. The sensitivity functions are given by:

$$
\Omega_A(\tilde{Z}) = \bar{\kappa}_{10} \exp\left(\frac{\tilde{A}^T}{\tilde{T} + \tilde{T}^*}\right)_{ss}
$$

$$
\Omega_T(\tilde{Z}) = \bar{\kappa}_{10} \frac{\tilde{A}^T}{(\tilde{T} + \tilde{T}^*)^2} \tilde{C} \exp\left(\frac{\tilde{A}^T}{\tilde{T} + \tilde{T}^*}\right)_{ss}
$$

$$
\Omega_B(\tilde{Z}) = \bar{\kappa}_{20} \exp\left(\frac{\tilde{B}^T}{\tilde{T} + \tilde{T}^*}\right)_{ss}
$$

$$
\Omega_{TB}(\tilde{Z}) = \bar{\kappa}_{20} \frac{\tilde{B}^T}{(\tilde{T} + \tilde{T}^*)^2} \tilde{C} \exp\left(\frac{\tilde{B}^T}{\tilde{T} + \tilde{T}^*}\right)_{ss}
$$

To evaluate the sensitivity functions, Equation (4-7), the steady state solution of the dimensionless nonlinear equations must be found. The steady state equations are obtained by setting the time derivatives in Equation (4-3) equal to zero; the result is

$$
\frac{\partial \tilde{C}A}{\partial \tilde{Z}} = -\bar{\kappa}_{10} \exp\left(\frac{\tilde{A}^T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C} \tilde{A}
$$

$$
\frac{\partial \tilde{C}B}{\partial \tilde{Z}} = \bar{\kappa}_{10} \exp\left(\frac{\tilde{A}^T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C} \tilde{A} - \bar{\kappa}_{20} \exp\left(\frac{\tilde{B}^T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C} \tilde{B}
$$

$$
\frac{\partial \tilde{T}}{\partial \tilde{Z}} = \bar{\kappa}_{10} \exp\left(\frac{\tilde{A}^T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C} \tilde{A} + \frac{b_2}{b_1} \bar{\kappa}_{20} \exp\left(\frac{\tilde{B}^T}{\tilde{T} + \tilde{T}^*}\right) \tilde{C} \tilde{B} + \tilde{\omega}(\tilde{Tc} - \tilde{T})
$$
These are the dimensionless form of Equation (3-21). The steady state solution is used to calculate the sensitivity functions. The sensitivity functions for the initial steady state are plotted as functions of reactor length in Figure 4-1.

To observe the effect of linearization on the system's response a step change is made in the feed conditions, and the nonlinear and the linear equations are solved to obtain the response of the system. Initially it is assumed that the feed conditions are: \( CA = 0.95; \) \( CB = 0.05; \) and \( T = 331.0 \) with \( TC = 316.0 \).

It should be mentioned at this point that the nonlinear equations can be linearized about any steady state profile and the initial profile does not have to be the optimal steady state. Therefore an initial steady state is used for the linearization which results in a more accurate approximation. For this reason \( TC = 316.0 \) was chosen rather than the optimal cooling water temperature, \( TC^* = 316.4 \). This shows how sensitive the linearization is to the change in \( TC \). In general it was observed that the accuracy of the linearization was a strong function of cooling water temperature, \( TC \), and to a lesser degree, dependent upon the magnitude of disturbance in the feed conditions.

Figure 4-2 shows the response of the system for a step disturbance in the feed conditions: \( CA = 0.65; \) \( CB = .35; \) and \( T = 300 \). The cooling water temperature, \( TC \), is kept constant at \( TC = 316.0 \). It is seen for the magnitude of the disturbances in the feed conditions the approximation is quite accurate. Therefore for our purpose, it can be assumed that the linearization of the nonlinear equations is a valid approximation.
FIGURE 4-1

SENSITIVITY COEFFICIENT

DIMENSIONLESS LENGTH

LEGEND
- RA(z)
- RT(z)
- R(z)
- AT(z)

Sensitivity Functions
CBQ = 0.05
TQ = 331.4
TC = 316.0
NON-LINEAR VS. LINEAR RESPONSE TO STEP CHANGE IN FEED
CA₀ = 0.65  CB₀ = 0.35  T₀ = 300.  TC = 316.0

FIGURE 4-2

LEGEND

- NON-LINEAR
- LINEAR

TIME (MIN.)

0.00  5.00  10.00  15.00  20.00  25.00

DIMENSIONLESS EXIT CONC. OF B
0.32  0.40  0.48  0.56  0.64  0.72  0.80  0.88

NON-LINEAR VS. LINEAR RESPONSE TO STEP CHANGE IN FEED
D. Laplace Transformation

In this section the Laplace transform of the system's equations are obtained in order to develop an approximate transfer function for the system. The input variables considered will be the cooling water temperature and feed concentration while the output will be the outlet concentration of B. Once this relationship is found, optimum control theory may be applied to obtain the optimal control. Since the Laplace transform is a linear operator, the development will commence with the linearized equations obtained in the previous section.

The Laplace transformation of a continuous and differentiable function, \( F(t,Z) \), which depends on both time and space is defined as:

\[
F(S,Z) = L[F(t,Z)] = \int_{0}^{\infty} F(t,Z) \exp(-tS)dt \quad (4-9)
\]

The Laplace transform of \( \frac{\partial F(t,Z)}{\partial t} \) can be calculated by using Equation (4-7) to obtain

\[
L\left[ \frac{\partial F(t,Z)}{\partial t} \right] = \int_{0}^{\infty} \frac{\partial F(t,Z)}{\partial t} \exp(-tS)dt \quad (4-10)
\]

The integrand of Equation (4-10) is integrated by parts:

\[
L\left[ \frac{\partial F(t,Z)}{\partial t} \right] = F(t,Z) \exp(-tS)\big|_{0}^{\infty} + S \int_{0}^{\infty} F(t,Z) \exp(-tS)dt \quad (4-11)
\]

The first term on the right hand side of Equation (4-11) is evaluated at its limits and Equation (4-9) is used to replace the second term. The result is

\[
L\left[ \frac{\partial F(t,Z)}{\partial t} \right] = SF(S,Z) - f(0,Z) \quad (4-12)
\]
The Laplace transform of the higher order partial derivatives of 
\( f(t, Z) \) with respect to \( t \) are obtained in a similar manner. The 
Laplace transform of the \( n^{th} \) order partial derivative is given by:

\[
L\left[ \frac{\partial^n f(t, Z)}{\partial t^n} \right] = s^n F(s, Z) - s^{n-1} F(0, Z) - s^{n-2} \frac{\partial f(0, Z)}{\partial t} - \ldots
\]

(4-13)

By differentiating Equation (4-9) with respect to \( Z \), the Laplace 
transform of \( f'(t, Z) \) is obtained as

\[
L \left[ \frac{\partial f(t, Z)}{\partial Z} \right] = \frac{\partial}{\partial Z} \int_0^\infty f(t, Z) \exp(-ts) dt = \int_0^\infty \frac{\partial f(t, Z)}{\partial Z} \exp(-ts) dt
\]

or

\[
L \left[ \frac{\partial f(t, Z)}{\partial Z} \right] = \frac{\partial F(s, Z)}{\partial Z}
\]

(4-14)

The Laplace transform of higher order partial derivatives with respect 
to \( Z \) are obtained in analogous manner. The Laplace transform of the 
\( n^{th} \) order partial of \( f(t, Z) \) with respect to \( Z \) is defined as

\[
L \left[ \frac{\partial^n f(t, Z)}{\partial Z^n} \right] = \frac{\partial^n F(s, Z)}{\partial Z^n}
\]

(4-15)

The above definitions are used to obtain the Laplace transforms 
of the linearized Equation (4-6). It can be assumed that the initial 
conditions on the dependent variables are zero and replace the 
variables with perturbed variables which are defined as the 
difference in the value of each variable and the corresponding 
steady state value of the same variable; the result is
The system of Equations (4-16) are coupled to one another and there is no simple way to obtain the relationship between the control, TC(t), and the outlet concentration of B. Therefore, another technique must be used to obtain the necessary relationship.

E. Frequency Response

To find the effect of control, TC(t), on the outlet concentration of B a frequency response technique is used. Experimental methods for obtaining the frequency response of a system are commonly based upon either pulse testing or sinusoidal perturbation. If the differential equations describing the system are available, these may also be used to obtain the frequency response of the system. This method is analytical and does not require the taking of experimental data.

The pulse test method is a black box technique which uses experimental data rather than the model equation. Initially it is assumed that the system is at steady state. It is then disturbed by a pulse input for a short period of time and the output of the system is measured; this gives the required experimental data. The
resulting time domain experimental data are transformed into the frequency domain by using Fourier analysis.

The method of sinusoidal input for obtaining the frequency response of a system also assumes that the system initially is at steady state. A sine wave of a given amplitude and frequency is applied to the system. By measuring the output it can be observed that the output is also sinusoidal in nature. If sufficient time is allowed the system would come to a new steady state which is a sine wave of a constant amplitude. By measuring the steady state amplitude and the phase angle of the output for each frequency, the frequency response of the system may be obtained.

All three methods were used to obtain the frequency response of the system. The pulse test method did not give satisfactory results. This was attributed to the initial discontinuity in the system and the small number of points in the output pulse. However, increasing the number of data points from 50 to 250 gave little improvement. Therefore, the pulse test method of obtaining the frequency response of the system was abandoned.

To obtain the frequency response of a distributed parameter system using the analytical method mentioned above, a transformed complex set of ordinary differential equations must be solved.

The set of partial differential equations are first transformed, as illustrated in Section D, into a set of ordinary differential equations. Upon substitution of $i\omega$ for the Laplace variable $S$, where $i$ is $\sqrt{-1}$ and $\omega$ is frequency, a complex set of ordinary differential equations is obtained. These may be solved by numerical methods to obtain the frequency response of the system. This technique is
First it is assumed that each variable is a complex number with a real and an imaginary part, or

\[ \frac{\text{CA}}{\text{CB}} = (\text{CAR}) + i(\text{CAi}) \]

\[ \frac{\text{CB}}{\text{TR}} = (\text{CBR}) + i(\text{CBi}) \]  \hspace{1cm} (4-17)

\[ \frac{T}{T} = (\text{TR}) + i(\text{Ti}) \]

These complex variables are substituted in the system of Equation (4-16). In addition, the substitution \( s = i\omega \) is also made. The result is

\[ \frac{\partial \text{CAR}}{\partial z} + i \frac{\partial \text{CAi}}{\partial z} = \omega \text{CAi} - \Omega_A \text{CAR} - \Omega_T \text{TR} - i(\omega \text{CAR} + \Omega_A \text{CAi} + \Omega_T \text{Ti}) \]

\[ \frac{\partial \text{CBR}}{\partial z} + i \frac{\partial \text{CBi}}{\partial z} = \Omega_A \text{CAR} + \omega \text{CBi} - \Omega_B \text{CBR} + (\Omega_T - \Omega_T) \text{TR} \]

\[ + i(\Omega_A \text{CAi} - \omega \text{CBR} - \Omega_B \text{CBi} + \Omega_T \text{Ti} - \Omega_T \text{Ti}) \]  \hspace{1cm} (4-18)

\[ \frac{\partial \text{TR}}{\partial z} + i \frac{\partial \text{Ti}}{\partial z} = \Omega_A \text{CAR} + \left(\frac{b^2}{b_1}\right)\Omega_B \text{CBR} - (\alpha - \Omega_T - \frac{b^2}{b_1} \Omega_T) \text{TR} + \omega \text{Ti} \]

\[ + \alpha \text{TC} + i \left[\Omega_A \text{CAi} + \left(\frac{b^2}{b_1}\right)\Omega_B \text{CBi} - (\alpha - \Omega_T - \frac{b^2}{b_1} \Omega_T) \text{Ti} - \omega \text{TR}\right] \]

To solve the system of Equations (4-18), the real and the imaginary part of left hand side of each equation separately is set equal to the real and the imaginary part of the right hand side of each equation.
respectively. The result is

\[ \frac{\partial CA}{\partial z} = \omega CA - \Omega_A CAR - \Omega_T TR \]

\[ \frac{\partial CA}{\partial z} = - (\omega CAR + \Omega_A CA + \Omega_T T) \]

\[ \frac{\partial CBR}{\partial z} = \Omega_A CAR + (\omega CB - \Omega_B CBR) + (\Omega_T - \Omega_{TB}) TR \]

\[ \frac{\partial CBi}{\partial z} = \Omega_A CA - \omega CBR - \Omega_B CB + \Omega_T T - \Omega_{TB} T \]  \hspace{1cm} (4-19)

\[ \frac{\partial TR}{\partial z} = \Omega_A CAR + \left( \frac{b_2}{b_1} \right) \Omega_B CBR - (\omega - \Omega_T) - \left( \frac{b_2}{b_1} \right) TR + uT + \omega T \]

\[ \frac{\partial Ti}{\partial z} = \Omega_A CA + \left( \frac{b_2}{b_1} \right) \Omega_B CB - (\omega - \Omega_T) - \left( \frac{b_2}{b_1} \right) T - uTR \]

The Equations (4-19) form a system of six ordinary linear differential equations which must be solved simultaneously.

To observe the effect of each input variable on the output, the real and the imaginary parts of all the other input variables and the imaginary part of the desired variable are set equal to zero; and the real part of the desired input variable is set to unity, because to obtain the effect of each input variable on the output independently. Then the frequency, \( \omega \), is varied and the system of equations are solved to obtain the real and the imaginary part of the output variable for the particular frequency. The real and the imaginary part of the output variable is combined in the following manner.
\[ CB = (CBR^2 + CBi^2)^{1/2} \]

Phase Angle of \( CB \) = \( \arctan \left( \frac{CBi}{CBR} \right) \) 

(4-20)

to obtain the magnitude and the phase angle of the output variable.

A fourth-order Runge-Kutta-Gill numerical integration program was used in integrating Equation (4-19).

The amplitude ratio and the phase angle of the output due to disturbance in the A concentration in the feed, \( CAO \), are shown in Figures 4-3 and 4-4. From Figure 4-3, it is seen that the exit concentration remains constant at its steady state value as the frequency is increased up to a break frequency of about \( \omega = 20 \). After this the amplitude ratio drops sharply as the frequency is increased.

The frequency response of the exit concentration of the desired product, B, due to disturbance in the control function, \( TC(t) \), is plotted in Figures (4-5) and (4-6). The amplitude ratio is shown in Figure 4-5 and the phase angle is plotted in Figure 4-6. From Figure 4-5 it is seen that the amplitude ratio remains constant as the frequency is increased up to \( \omega = 1.0 \). Then it starts decreasing but the decrease is not as sharp as the one in Figure 4-3. A hump appears in the response around \( \omega = 7.0 \). This is called a resonance peak. There are also other smaller resonance peaks at higher frequencies. The presence of resonance peaks in the frequency response of a distributed parameter systems is a distinct characteristic of these systems.
FREQUENCY RESPONSE OF B EXIT CONCENTRATION DISTURBANCE IN CA0

FIGURE 4-3
FREQUENCY RESPONSE OF B EXIT CONCENTRATION DISTURBANCE IN CA₀

FIGURE 4-4
FREQUENCY RESPONSE OF B EXIT CONCENTRATION DISTURBANCE IN CONTROL TC(T)

FIGURE 4-5
FREQUENCY RESPONSE OF B EXIT CONCENTRATION DISTURBANCE IN CONTROL TC(T)

FIGURE 4-6

DIMENSIONLESS FREQUENCY W

PHASE ANGLE (D) $\times 10^1$

$-120.00$ $-180.00$ $-240.00$ $-280.00$
The method of sinusoidal input was also used to obtain the frequency response of the system. The nonlinear partial differential equations were forced by a sinusoidal $\text{TC}(t)$ and solved numerically. The results were in close agreement with those which were obtained using the analytical technique. This also indicated the validity of the linearization of the nonlinear equations.

Comparing all the three methods, it could be concluded that the analytical method was the most efficient means of obtaining the frequency response of the system. This method required a short period of computation and it was relatively straightforward. On the other hand, the sinusoidal input method needed longer computation time because the system had to reach to a new steady state before the output amplitude ratio could be measured; also phase angle could not be measured easily. There were some problems associated with the amplitude of the input sine wave; short amplitudes resulted in short output amplitude and the steady state could not be observed easily. For the large input amplitude the system did not come to the steady state in a short period of time. Therefore, it is recommended to use the analytical method to obtain the frequency response of this type system.

F. **The System's Transfer Function**

The transfer function concept is one of the basic elements of the classical control theory. The transfer function of a system is defined as the ratio of the Laplace transform of the output to the Laplace transform of the input. If the output of the system (in the Laplace domain) is denoted by $\text{C}(\text{S})$; and the input of the system
by $M(S)$; then the transfer function of the system, $G(S)$, is defined as

$$G(S) = \frac{C(S)}{M(S)}$$  \hspace{1cm} (4-21)

Once the transfer function of the system is obtained, many control problems, such as stability and optimal control, can be easily solved.

One may determine an approximate transfer function of a system knowing the frequency response of the system. First a model for the transfer function is assumed. Usually this is one which can be readily inverted into time domain and includes terms characteristic of the observed frequency response of the particular system. The chosen model will contain a number of parameters whose numerical values are determined by the statistical methods described below.

One would like to select these values such that a "best" fit is obtained in the time domain. The minimization of the integral of Equation (4-22) is commonly used

$$ISE = \int_{0}^{\infty} [f(t,Z)-h(t,Z)]^2 dt$$  \hspace{1cm} (4-22)

where

$f(t,Z) = \text{the actual time response of the system}$

$h(t,Z) = \text{the time response of the transfer function}$

Schnelle, utilizing Parseval's theorem, has shown that the frequency domain equivalent of Equation (4-22) is given by:

$$ISEF = \int_{0}^{\infty} \left[ G^2 - 2GHCos(\Theta - \Phi) + H^2 \right] d\omega$$  \hspace{1cm} (4-23)
where

\[ G = |F(\omega, Z)| = \text{actual magnitude of system frequency response} \]

\[ H = |h(\omega, Z)| = \text{the magnitude of the approximate response obtained from the transfer function.} \]

\[ \Theta = \text{actual phase angle of system frequency response} \]

\[ \Phi = \text{approximate phase angle obtained from the transfer function response.} \]

Planchard and Gonzalez (26), have shown the following transfer function

\[ G(S) = \frac{1-XKP \exp(-\tau_o S)}{(1+\tau_1 S)(1+\tau_2 S)} \]  

(4-24)

where

\[ XKP = 1 - \text{steady state gain} \]

\[ \tau_o = \text{dead time} \]

\[ \tau_1, \tau_2 = \text{time constants.} \]

gives good time domain fit to the response of heat exchangers. They have also shown for the type of frequency response of Figures 4-3 and 4-4 the following transfer function is a suitable one:

\[ G(S) = GN \frac{\exp(-\tau_0 S)}{(1+\tau_1 S)(1+\tau_2 S)} \]  

(4-25)

where

\[ GN = \text{steady state gain.} \]

To obtain the best parameters for Equation (4-24) and (4-25), starting values of the parameter for \( \tau_o, \tau_1, \) and \( \tau_2 \) were chosen. Values of \( GN \) and \( XKP \) are obtained by extrapolating the system's frequency response to zero frequency. Since the amplitude ratio at this frequency corresponds to \( GN \). Then the frequency response of the
transfer function is calculated and the integrand of Equation (4-23) is evaluated. To minimize the integrand of Equation (4-23), a minimization program due to Powell (57) was used. Pattern search (79) was also used, but the routine was not as efficient or as rapidly convergent as the Powell method.

Although, Equation (4-25) represented the frequency response of Figures 4-3 and 4-4 more accurately than Equation (4-24), the final analysis showed the system obtained from the transfer function was unstable. The unstability was mainly due to the small time constants \( \tau_1 = \tau_2 = 0.040 \) calculated for Equation (4-25). Since the purpose of this investigation was not to find an accurate representation of the frequency response of the system; rather, it was intended to obtain the optimal control of a distributed parameter system using transfer function concept; therefore, Equation (4-24) was used to fit the frequency response of the system with disturbance in CAO and all other input variables.

Optimal parameters for the transfer functions were obtained by selecting several widely different starting points in the search. In most cases the same optimal parameters were obtained. Table 3 lists the optimal parameters for each transfer function using Equation (4-24).
TABLE 3.

Optimal Parameters of $G(S)$ Obtained in the Frequency Domain

<table>
<thead>
<tr>
<th>Transfer Function</th>
<th>$T_0$</th>
<th>$T_1$</th>
<th>$T_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{CB(S,1)}{CAO(S)}$</td>
<td>1.061</td>
<td>.625</td>
<td>.626</td>
</tr>
<tr>
<td>$\frac{CB(S,1)}{CBO(S)}$</td>
<td>1.055</td>
<td>.673</td>
<td>.673</td>
</tr>
<tr>
<td>$\frac{CB(S,1)}{TO(S)}$</td>
<td>1.028</td>
<td>.803</td>
<td>.804</td>
</tr>
<tr>
<td>$\frac{CB(S,1)}{TC(S)}$</td>
<td>.935</td>
<td>.545</td>
<td>.547</td>
</tr>
</tbody>
</table>

The actual frequency response of the system and the response obtained from the transfer function due to disturbance in CAO are plotted in Figures 4-7 and 4-8. Those due to disturbance in the control, $TC(t)$, are plotted in Figures 4-9 and 4-10. In each case the transfer functions gave excellent fit to the frequency responses at low frequencies. The fitness was not as good in the middle frequencies, and quite poor in the high frequency range. However, for all practical purposes, only low and middle range frequencies are used in actual cases. Therefore, it can be assumed that the transfer function representation of the system is an adequate representation.

Since the optimal control calculations are carried out in the time domain, rather than the frequency domain; it is desirable to compare the time domain response of the linearized system and the
FREQUENCY RESPONSE OF B EXIT CONCENTRATION

\[ G_1(S) = \frac{C_B(S, 1)}{C_{A0}(S)} \]

LEGEND

□ ACTUAL

\( G_1(S) \)

FIGURE 4-7
FREQUENCY RESPONSE OF B EXIT CONCENTRATION

\[ G_1(S) = \frac{CB(S, 1)}{CA_0(S)} \]

**Legend**

- □: AC'UAL
- ○: G1(S)

**Figure 4-8**

**Dimensionless Frequency W**

**Phase Angle**

-240.0
-180.0
-120.0
-60.0
0.0

**Frequency**

\[ 10^{-5} \]
\[ 10^{-2} \]
\[ 10^{-1} \]
\[ 10^{0} \]
\[ 10^{1} \]
\[ 10^{2} \]
FREQUENCY RESPONSE OF B EXIT CONCENTRATION

\[ G_2(S) = \frac{C_B(S, 1)}{T_C(S)} \]

LEGEND

\[ \square \] ACTUAL

\[ \circ \] \( G_2(S) \)

FIGURE 4-9
FREQUENCY RESPONSE OF B EXIT CONCENTRATION
\[ G_2(S) = \frac{C_0'(S, 1)}{C_0(S)} \]

LEGEND
- A - TUAL
- G_2(S)

FIGURE 4-10

PHASE ANGLE

-240.00
-160.00
-80.00
0.00
80.00
160.00
240.00

DIMENSIONLESS FREQUENCY \( \omega \)
response of the transfer function. A step disturbance of magnitude $H$ in control $TC(t)$ is introduced into the system; then the linearized equations are solved to obtain the response of the system. The transfer function response of the system is computed by obtaining the inverse Laplace transform of the transfer function as follows

$$G(s) = \frac{CB(S,1)}{TC(S)} = \frac{1-XKP e^{-\tau o s}}{(1+\tau_1 S)(1+\tau_2 S)}$$

(4-26)

$TC(S)$ in Equation (4-26) is replaced with its Laplace transform:

$$TC(S) = \frac{H}{S}$$

(4-27)

Then

$$CB(S,1) = \frac{H}{S} \left[ \frac{1-XKP e^{-\tau o s}}{(1+\tau_1 S)(1+\tau_2 S)} \right] = \frac{H}{S(1+\tau_1 S)(1+\tau_2 S)} - \left[ \frac{H}{S(1+\tau_1 S)(1+\tau_2 S)} \right] XKP e^{-\tau o s}$$

(4-28)

The time domain response is obtained by taking the inverse Laplace transform of Equation (4-28):

$$CB(t,1) = H \left[ \frac{1}{\tau_2} \frac{1}{\tau_1} \right] \exp\left( -\frac{t}{\tau_1} \right) - \frac{H}{\tau_2} \left[ \frac{1}{\tau_1} \right] \exp\left( -\frac{t}{\tau_2} \right)$$

(4-29)
TIME DOMAIN RESPONSE OF B EXIT CONCENTRATION
STEP DISTURBANCE IN TC(T)

LEGEND
□ LINEARIZED EQUATIONS
○ TRANSFER FUNCTION

DIMENSIONLESS CONCENTRATION
0.70
0.72
0.74
0.76
0.78
0.80

TIME (MIN.)
0.00
5.00
10.00
15.00
20.00
25.00

FIGURE 4-11
where

\[ X_{KP} = \text{steady state gain} \]

\[ U(t-t_0) = \text{a unit delay function} \]

To obtain \( X_{KP} \) in Equation (4-29) the limit of (4-29) is taken as time, \( t \), approaches to infinity.

\[ CB(\infty,1) = H - X_{KP}[H] \]  \hspace{1cm} (4-30)

\[ X_{KP} = \frac{H - CB(\infty,1)}{H} \]  \hspace{1cm} (4-31)

\( CB(\infty,1) \) is obtained from the solution of the linearized equation, after a step disturbance of magnitude \( H \) in the control function \( TC(t) \).

Figure 4-11 shows the results of a step disturbance in the control with magnitude \( H \) equal to the steady state value of \( TC_{ss} \).

It can be seen that the both responses are in close agreement despite the rather poor frequency response fit at high frequencies. Therefore, it can be concluded that the transfer function \( G_1(S) \), Equation (4-24) gives an adequate representation of the system's response in the time domain.
A. Introduction

The concept of state is the basic element of modern control theory. The state of a system is defined as sufficient information about the system at some time $t_0$; this information, together with the subsequent input to the system, are sufficient to describe the future behavior of the system subsequent to $t \geq t_0$ (43).

In this chapter the optimal control of the system using the state concept will be obtained. By using the transfer function representation of the system as determined in the preceding chapter, state variable equations are obtained. Then, the minimum principle for the optimal control of the lumped parameter systems is used to find the optimal control of the approximate system. The calculated optimal control is then applied to the original system of nonlinear equations and the yield is obtained. If the approximations which have been made so far are valid, then the obtained yield must be in the neighborhood of the yield using the optimal control theory for distributed parameter systems. Since it is desired to observe whether this method of obtaining the optimal control of a distributed parameter system is valid, the only disturbance in the feed which will be considered is due to the change in the concentration of reactant A. In other words, it is assumed that the concentration of B in the feed remains at $C_B = 0.05$ and the feed temperature is kept constant at $T = 331.4$. 
B. **State Representation of the System**

Using the parameters obtained in the previous section the following transfer functions are defined:

\[
G_1(S) = \frac{CB(S,1)}{CAO(S)} = \frac{1 - XKP \exp(-1.061S)}{(1 + .626S)(1 + .625S)}
\]

\[
G_2(S) = \frac{CB(S,1)}{TC(S)} = \frac{1 - XKP \exp(-0.935S)}{(1 + .545S)(1 + .547S)} \quad (5-1)
\]

or for the general case

\[
G_1(S) = \frac{CB(S,1)}{CAO(S)} = \frac{1 - XKP \exp(-\tau_{01}S)}{(1 + \tau_1S)(1 + \tau_2S)}
\]

\[
G_2(S) = \frac{CB(S,1)}{TC(S)} = \frac{1 - XKP \exp(-\tau_{02}S)}{(1 + \tau_3S)(1 + \tau_4S)} \quad (5-2)
\]

Assuming \(CAO(S)\) is the disturbance variable and \(TC(S)\) is the manipulated variable; then, the exit concentration could be related to the disturbance and the manipulated variables in the following manner:

\[
CB(S,1) = G_1(S) \cdot CAO(S) + G_2(S) \cdot TC(S) \quad (5-3)
\]

or

\[
CB(S,1) = \frac{1 - XKP \exp(-\tau_{01}S)}{(1 + \tau_1S)(1 + \tau_2S)} \cdot CAO(S) + \frac{1 - XKP \exp(-\tau_{02}S)}{(1 + \tau_3S)(1 + \tau_4S)} \cdot TC(S) \quad (5-4)
\]

It should be noted that all the variables appearing in Equation (5-4) are perturbed variables; in other words, they are deviations from the steady state value of each variable.
To obtain the state representation of (5-4), two state vectors, \( X_1 \) and \( X_3 \) are introduced. The state vectors are defined as

\[
X_1 = \frac{1 - X_0 \exp(-\tau_{01} S)}{(1 + \tau_1 S)(1 + \tau_2 S)} \text{CAO}(S)
\]

\[
X_3 = \frac{1 - X_0 \exp(-\tau_{02} S)}{(1 + \tau_3 S)(1 + \tau_4 S)} \text{TC}(S)
\]

Substitution of the system of Equations (5-5) in (5-4), results in

\[
C_B(S, 1) = X_1 + X_3 \quad (5-6)
\]

By taking the inverse Laplace transform of Equation (5-5), the time domain response of the approximate system is obtained as the solution to

\[
\frac{d^2 X_1}{dt^2} + \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} \frac{dX_1}{dt} + \frac{X_1}{\tau_1 \tau_2} = \frac{\text{CAO}(t) - X_0 \text{CAO}(t - \tau_{01})}{\tau_1 \tau_2}
\]

\[
\frac{d^2 X_3}{dt^2} + \frac{\tau_3 + \tau_4}{\tau_3 \tau_4} \frac{dX_3}{dt} + \frac{X_3}{\tau_3 \tau_4} = \frac{\text{TC}(t) - X_0 \text{TC}(t - \tau_{02})}{\tau_3 \tau_4}
\]

Now, the following state variables are defined

\[
x_1 = X_1 \quad \frac{dx_1}{dt} = \frac{dx_1}{dt}
\]

\[
x_2 = X_1 = \frac{dx_1}{dt}
\]

\[
x_3 = X_3 \quad \frac{dx_3}{dt} = \frac{dx_3}{dt}
\]

\[
x_4 = X_3 = \frac{dx_3}{dt}
\]
The state variables are introduced in the system of Equation (5-7), the result is:

\[
\begin{align*}
\dot{x}_1 &= x_2 \\
\dot{x}_2 &= -\frac{\tau_1 + \tau_2}{\tau_1 \tau_2} x_2 - \frac{1}{\tau_1 \tau_2} x_1 + g_1(t) \\
\dot{x}_3 &= x_4 \\
\dot{x}_4 &= -\frac{\tau_3 + \tau_4}{\tau_3 \tau_4} x_4 - \frac{1}{\tau_3 \tau_4} x_3 + g_2(t)
\end{align*}
\]

(5-9)

where

\[
\begin{align*}
g_1(t) &= \frac{C_A(t) - X_K P G_A(t - \tau_{01})}{\tau_1 \tau_2} \\
g_2(t) &= \frac{C_C(t) - X_K P T_C(t - \tau_{02})}{\tau_3 \tau_4}
\end{align*}
\]

(5-10)

The exit concentration of the desired product, B, is related to the state variables by

\[C_B(t, 1) = x_1 + x_3\]

(5-11)

C. Computational Scheme

Assume the tubular reactor has been operating at steady state; at time \(t = 0\) the feed is subject to a step disturbance in composition. It is desired to find the optimal cooling water temperature such that, the cumulative yield of the desired product, B, is maximized during a specified time interval, \(t_0 \leq t \leq t_f\). The dynamics of the reactor are approximated by the system of Equations (5-9).

As in the case for the distributed parameter system (Chapter III),
an objective function must be defined. Since the cumulative yield of B is desired, a suitable objective function would be

\[ J = - \int_0^{t_f} CB(t,1)dt \] (5-12)

Minimization of (5-12) is equivalent to the maximization of the cumulative yield of B. Using Equation (5-12) as the objective function, resulted in a trivial solution. Therefore, rather than using (5-12) as the objective function, a new objective function is defined:

\[ J = - \int_0^{t_f} CB^2(t,1)dt \] (5-13)

Minimizing Equation (5-13) would result in the maximization of the cumulative yield of B, during the time interval \( 0 \leq t \leq t_f \).

Now, Equation (5-11) is substituted into (5-13), the result is

\[ J = - \int_{t_0}^{t_f} (x_1 + x_3)^2 dt \] (5-14)

The hamiltonian function is defined as

\[ H = \langle \tilde{P} \cdot \tilde{F} \rangle = P_1x_2 + P_2(- \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} x_2 - \frac{1}{\tau_1 \tau_2} x_1 + g_1(t)) + P_3x_4 \]

\[ + P_4(- \frac{\tau_3 + \tau_4}{\tau_3 \tau_4} x_4 - \frac{1}{\tau_3 \tau_4} x_3 + g_2(t)) - (x_1 + x_3)^2 \] (5-15)

where

\[ \tilde{P} = \text{The vector of adjoint variables} \]
\( \mathbf{F} \) = A column vector with each element being the right hand side of Equation (5-9)

Using the minimum principle for the optimal control of lumped parameter systems, the system of adjoint variables are obtained as:

\[ \mathbf{p} = - \frac{\partial H}{\partial \mathbf{x}} \]

\[ \frac{dp_1}{dt} = - \frac{\partial H}{\partial x_1} = 2(x_1 + x_3) + \frac{1}{\tau_1 \tau_2} p_2 \]

\[ \frac{dp_2}{dt} = - \frac{\partial H}{\partial x_2} = -p_1 + \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} p_2 \quad (5-16) \]

\[ \frac{dp_3}{dt} = - \frac{\partial H}{\partial x_3} = 2(x_1 + x_3) + \frac{1}{\tau_3 \tau_4} p_4 \]

\[ \frac{dp_4}{dt} = - \frac{\partial H}{\partial x_4} = -p_3 + \frac{\tau_3 + \tau_4}{\tau_3 \tau_4} p_4 \]

The control of the system is achieved by manipulation of \( g_2(t) \) only, because once the step change has been made \( g_1(t) \) is specified by the forcing function (feed composition). Therefore, the Hamiltonian (5-15) must be minimized with respect to the choice of control, \( g_2(t) \).

Since the Hamiltonian is linear with respect to the control, \( g_2(t) \); setting its partial with respect to \( g_2(t) \) equal to zero will result in a trivial solution of \( g_2(t) = 0 \) which is not acceptable. In order to minimize \( H \) with respect to control, \( g_2(t) \), it is necessary to minimize the terms in \( H \) which contain \( g_2(t) \). Thus, the optimal control is obtained by minimizing the product of
P_4 g_2(t) in Equation (5-15); this purpose is achieved if the control, g_2(t), is changed according to the sign of P_4. This requires setting the control to its highest values whenever P_4 is negative and to its lowest value at other times. Using this strategy will result in a control which is either $+\infty$ or $-\infty$ which is not practical. Therefore, an upper and lower limit for the control, g_2(t), is assumed and a search will be done to find the limits which maximize the cumulative yield of the desired product. Assuming there are constraints on g_2(t), which are defined by

$$GL \leq g_2(t) \leq GH$$  \hspace{1cm} (5-17)$$

then, to minimize $P_4 g_2(t)$, GL is the control whenever $P_4$ is positive; and GH is the control whenever $P_4$ is negative. In other words, the optimal control strategy is defined as:

$$g_2^*(t) = \begin{cases} GH & \text{if } P_4(t) < 0 \\ GL & \text{if } P_4(t) \geq 0 \end{cases}$$  \hspace{1cm} (5-18)$$

Once the optimal control strategy, $g_2^*(t)$, has been established; Equation (5-10) is used to obtain the optimal cooling water temperature.

To solve the system of Equations (5-9) and (5-16) eight initial conditions are needed. The initial conditions on the state variables are specified by the fact that initially the system is at steady state, therefore

$$CB(0,1) = \frac{dCB(0,1)}{dt} = \frac{d^2CB(0,1)}{dt^2} = \frac{d^3CB(0,1)}{dt^3} = 0$$  \hspace{1cm} (5-19)$$
Equations (5-9), (5-11), and (5-19) are combined to obtain the initial conditions for the state variables as the solution to the following system of four linear equations in four unknowns:

\[
\begin{align*}
\frac{1}{\tau_1 \tau_2} x_1 + \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} x_2 + \frac{1}{\tau_3 \tau_4} x_3 + \frac{\tau_3 + \tau_4}{\tau_3 \tau_4} x_4 &= g_1(t) + g_2(t)(-\text{sign} P_4) \\
\frac{\tau_1 + \tau_2}{(\tau_1 \tau_2)^2} x_1 + \left[\frac{(\frac{\tau_1 + \tau_2}{\tau_1 \tau_2})^2 - \frac{1}{\tau_1 \tau_2}}{\frac{1}{\tau_1 \tau_2}}\right] x_2 + \frac{\tau_3 + \tau_4}{(\tau_3 \tau_4)^2} x_3 + \left[\frac{(\frac{\tau_3 + \tau_4}{\tau_3 \tau_4})^2 - \frac{1}{\tau_3 \tau_4}}{\tau_3 \tau_4}\right] x_4 &= \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} g_1(t) + \frac{\tau_3 + \tau_4}{\tau_3 \tau_4} g_2(t)(-\text{sign} P_4)
\end{align*}
\]

(5-20)

The initial conditions on the adjoint variables are unknown, but the final conditions are specified by the transversality conditions as

\[
P_1(t_f) = P_2(t_f) = P_3(t_f) = P_4(t_f) = 0
\]

(5-21)

Therefore, to obtain the optimal control the following procedure, Figure 5-1, is followed: the initial values of the adjoint variables are guessed; the system of Equations (5-20) are solved to obtain the initial conditions on the state variables. Having specified the eight initial conditions, the state and the adjoint equations are integrated forward in time up to time \( t = t_f \). The obtained final values of the adjoint variables are compared to those of (5-21), if the results are within a prescribed tolerance; then the assumed
Figure 5-1 Logic Diagram for Optimal Feedforward Control of the Approximate System
initial conditions on the adjoint variables are correct and the obtained $g_2(t)$ is the optimal control strategy, $g_2^*(t)$. Then, Equation (5-10) is used to calculate the optimal cooling water temperature. If the final values of the adjoint variables are not within the required tolerance, new values for the initial conditions on the adjoint variables are assumed and the whole process is repeated again until a satisfactory result is achieved.

D. Actual vs. Approximate Control

The actual optimal control of the reactor was obtained using the optimal control theory for distributed parameter systems, as was described in the Chapter III. Initially the feed conditions chosen were: $CAO = 0.95; CBO = 0.05$; and $TO = 331.4$. The cooling water temperature was the optimal steady state temperature; $TC = 316.4$. At time $t = 0^+$, the inlet load variables were changed to $CAO = 0.65$, $CBO = 0.05$, and $TO = 331.4$. Pattern search was used to obtain the new optimal steady state cooling water temperature. $TC_{ss}$ was $325.40K$. The initial steady state concentrations and temperature profiles are those of Figures 3-2, 3-3. The new steady state profiles of concentrations and temperature are plotted in Figures 5-2 and 5-3.

The cumulative yield of the desired product $B$ with no control action, using the old steady state cooling water temperature, $TC = 316.4$, was $11.584 \text{ g.mole/liter}$. Instantaneous application of the new steady state cooling water temperature, $TC = 325.40K$, resulted in a yield of $12.861 \text{ g.mole/liter}$ of the desired product. The optimal control is plotted in Figure 5-4; it drops from the
NEW OPTIMAL STEADY STATE SOLUTION AFTER STEP DISTURBANCE IN FEED CONCENTRATION PROFILE

LEGEND

○ CA(Z)
○ CB(Z)

FIGURE 5-2

CONCENTRATION G-MOLE/LITER

0.60
0.50
0.40
0.30
0.20
0.10
0.00

0.00 0.20 0.40 0.60 0.80 1.00

REACTOR LENGTH
NEW OPTIMAL STEADY STATE SOLUTION AFTER STEP DISTURBANCE IN FEED TEMPERATURE AND CONTROL PROFILE

LEGEND
M T(Z) O TC

FIGURE 5-3

TEMPERATURE (°K)
344.00
340.00
336.00
332.00
328.00
324.00
320.00

REACTOR LENGTH
0.00 0.20 0.40 0.60 0.80 1.00
initial steady state value, $TC = 316.4^\circ K$, to $TC = 309^\circ K$; it starts rising in a zigzag fashion. The optimal control then oscillates about the steady state with a sharp hump one residence time before the final time, $t_f = 25$ minutes. Instantaneous optimal yield due to the application of the optimal control is plotted in Figure 5-5. The exit concentration remains relatively constant up to time $t = 10$ min.; then, there is a sharp drop in the instantaneous yield, after which it starts rising rapidly to the new steady state exit concentration and remains constant at this value up to the final time. Instantaneous yields with the applications of the new steady state and the optimal control are plotted in Figure 5-6. The lower yield due to the instantaneous application of the steady state control is explained by the early drop of the instantaneous yield; this justifies the use of the optimal control, rather than the new steady state control. The cumulative optimal yield was 13.246 g.mole/liter.

To obtain the optimal control from the transfer functions six unknown variables must be found. These consist of the four initial conditions on the adjoint variables and the high and low control limits, GH and GL. The optimal values of GH and GL are those which result in the maximum yield of the desired product, B. A search to obtain the six unknown variables simultaneously proved to be ineffective. Both pattern search and Powell's method were used separately with no successful results. Subsequently, Golden search was used to obtain the optimal GH and GL, one variable at a time; and Powell's method was used to calculate the initial values of the adjoint variables. This procedure proved to be most effective;
OPTIMAL CONTROL AFTER STEP DISTURBANCE
COOLING WATER TEMPERATURE

Figure 5-4
OPTIMAL YIELD AFTER STEP DISTURBANCE
INSTANTANEOUS YIELD

FIGURE 5-5
OPTIMAL YIELD AFTER STEP DISTURBANCE
NEW STEADY STATE CONTROL VS. OPTIMAL CONTROL

LEGEND

OPTIMAL CONTROL
NEW STEADY STATE CONTROL

FIGURE 5-6
because a series of solutions were obtained, relating the initial conditions on the adjoint variables to GH and GL. Therefore, a table could be constructed that relates the non-optimal values of GH and GL to the initial conditions on the adjoint variables. Once the values of GH and GL are specified by the constraints; by referring to the table, the initial condition on the adjoint variables are obtained easily.

The optimal values of GH and GL were found to be $GH^* = 0.2324$ and $GL^* = .1652$. The optimal $g_2(t)$ was substituted in Equation (5-10) to obtain the optimal cooling water temperature, $TC(t)$. The calculated optimal control from the approximate system is plotted in Figure 5-7 and is compared to the optimal control, using the optimal control theory for the distributed parameter system, in Figure 5-8. The approximate control rises from the old steady state, $TC = 316.4$, to $TC = 321.08$ and remains constant at this value for two minutes; then it increases to $TC = 322.98$ and for the next seven minutes is held at this temperature. After this, another similar cycle begins, the process is repeated until the final temperature, $TC = 325.98$, is reached.

The cumulative yield, using the approximate control, is 13.067 g.mole/liter which is higher than the yield using the new steady state control, but is lower than the optimal yield. Table 4 shows the yield with different controls.
OPTIMAL CONTROL AFTER STEP DISTURBANCE
APPROXIMATE CONTROL

FIGURE 5-7
OPTIMAL CONTROL AFTER STEP DISTURBANCE
APPROXIMATE VS. OPTIMAL CONTROL

LEGEND
• APPROX. CONTROL  ○ OPTIMAL CONTROL

FIGURE 5-8
From Table 4 it is seen, taking no new control action, after the step disturbance, would result in a poor yield with high deviation from the optimal yield; the yield is improved by the instantaneous application of the new steady state control. The application of the optimal control from the approximate system results in a higher yield from either the old or the new steady state control with a low deviation of 1.3 per cent from the optimal yield. The instantaneous yields using the optimal control and the approximate control are plotted in Figure 5-9. Except for the first ten minutes, the two curves follow one another closely. The decrease in the yield using the approximate system, is mainly due to the early drop in the instantaneous yield; the drop is not as much as the drop using the new steady state control which explains the improvement over the cumulative yield using the new steady state control.

### E. Advantages and Disadvantages of the Approximate Control

Comparing the optimal and the approximate control (Figure 5-8), from the industrial viewpoint, it can be concluded that the implementation of the approximate control is more practical than that

<table>
<thead>
<tr>
<th>Type of Control</th>
<th>Cumulative Yield g.mole/liter</th>
<th>% Deviation From the Optimal Yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>Old Steady State</td>
<td>11.584</td>
<td>12.5</td>
</tr>
<tr>
<td>New Steady State</td>
<td>12.861</td>
<td>2.9</td>
</tr>
<tr>
<td>Optimal Control</td>
<td>13.246</td>
<td>0.0</td>
</tr>
<tr>
<td>Approximate Control</td>
<td>13.067</td>
<td>1.3</td>
</tr>
</tbody>
</table>
OPTIMAL YIELD AFTER STEP DISTURBANCE
APPROXIMATE VS. OPTIMAL CONTROL

LEGEND

Approx. Control
Optimal Control

FIGURE 5-9

YIELD G-MOLE/LITER

TIME (MIN.)
of the optimal control. Improvement of the cumulative yield also justifies the use of the approximate control, rather than the new steady state control. Another advantage of the approximate control and system is in design of controllers for the systems. Having the system's transfer function makes it relatively easy to design a stable controller, without disturbing the actual system. The most important property of the approximate system is that for any disturbance in the feed conditions all that is needed for the calculation of the optimal control is to find the new initial conditions on the adjoint variables and the new optimal GH and GL. If the optimal control theory for the DPS was to be used the complete process of calculations of the optimal control would have had to be repeated; this is not desirable from the practical standpoint.

The main disadvantage of obtaining the approximate control, besides resulting in a lower cumulative yield than the optimal yield, is that there are constraints on the control. As it was seen in the previous section the constraints were assumed to be on \( g_2(t) \) and there was no particular problem associated with treating the constraints. However, if the constraints are on the control, rather than \( g_2(t) \), there is no direct method of transforming the constraint on TC\((t)\) to the constraint on \( g_2(t) \). One possible solution to this problem is using trial and error technique. For a given set of constraints on TC\((t)\), a set of constraints on \( g_2(t) \) is assumed and the optimal TC\((t)\) is obtained. If the obtained optimal TC\((t)\) does not violate the constraints on the control, then the assumed constraints on \( g_2(t) \) were satisfactory; if not, a new set of constraints
are selected and the process is repeated until a satisfactory result is achieved.

Although the approximations which were used in the previous chapter were not as accurate as desired, the results of this chapter demonstrate the approach which was used to obtain the optimal control of the system was essentially correct. It can be concluded that a more exact representation of the system, along with the method of this chapter, would result in a better control and higher yield.
A. Introduction

So far only the optimal feedforward control of the distributed parameter system has been considered. The optimal control functions that have been developed are all based on the measured incoming disturbances and the initial operating conditions. The main disadvantage of using this type control is that the controller has no knowledge of its effects on the exit concentration of the desired product. Another disadvantage of the feedforward control is that other disturbances aside from those which have been considered are present. In this case the controller will not take any control action to eliminate the effects of these additional disturbances on the system. Also, the design of feedforward controllers requires precise knowledge of the system, and the exact effect of each variable on the system. Therefore, from an engineering point of view, stand-alone feedforward control of a system is not desirable except in a few instances.

An optimal control which is a function of both the state of the system and the load variables, is called optimal feedback control. A control function which is a function of state variables is called a control law. Design of a feedback control system does not require the precise knowledge of the system's behavior nor does it require the measurement of all the load variables.

In contrast to a lumped parameter system, the determination of the state variables at the exit point of a DPS is not sufficient in
calculation of the control law. This is due to the fact that the state variables for a DPS are functions of both time and space coordinate. Therefore, the location and the number of feedback sensors must be specified in order to obtain a realistic control law.

B. Formulation and Scheme of Solution

Most of the literature in the field of optimal feedback control of distributed parameter systems are based on linear systems with quadratic performance indices. Design of feedback control of non-linear DPS was discussed by Paradis and Perlmutter (53), who considered the control of a non-isothermal tubular reactor. As the objective function, they considered minimization of the deviation of the instantaneous state from the desired state. Seinfeld and Kumar (62), obtained the optimal open-loop control for parabolic and first order hyperbolic system. Then by using a least square approximation derived techniques for the synthesis of sub-optimal feedback control. Koivo and Kruh (37) also used the same concept to obtain the approximately optimal feedback controllers for one dimensional heat conduction system. A gradient technique was used to obtain the best controller parameters and a search technique was used to find the optimal positions of the feedback sensors. The basic assumption in the latter two papers was the existence of the open-loop, optimal feedforward control and the corresponding optimal state.

Since our objective is to maximize the cumulative yield during a certain time interval, the knowledge of the open-loop optimal control of the system is not required to obtain the optimal feedback
control. As previously was mentioned, the cost function is defined as

\[ J = \text{cost} = -\int_{0}^{T} CB(t,1) dt \quad (6-1) \]

Minimization of Equation (6-1) is equivalent to maximizing the cumulative yield of the desired product, B. It is desired to obtain an optimal feedback controller which results in a cumulative yield, approximately equal to one obtained using the optimal feedforward control.

To obtain the optimal feedback control, a mathematical model for the controller is assumed. This model, depending on the number of feedback sensors, will contain one or more parameters. Then, a direct search is used to find the optimal parameters and the optimal locations of the feedback sensors.

C. Single Feedback Sensor

The simplest type of feedback controller is one which has an output proportional to input, or for our case

\[ TC(t) = K(Z) CB(t,Z) \quad (6-2) \]

where K(Z) is the proportionality constant (the gain) of the controller. The gain could also be a function of time, but from the practical standpoint a variable gain is not desirable. It is obvious that using Equation (6-2) as the control algorithm, would result in obtaining a controller with a highly fluctuating output. Therefore, to reduce the output fluctuations the following control algorithm is defined
where $C(Z)$ is a constant temperature cooling water which is mixed with a calculated amount of another stream of cooling water with temperature equal to $K(Z)CB(t,Z)$ and the result is the overall cooling water temperature $TC(t)$. The main advantage of using Equation (6-3) rather than (6-2), as the control algorithm is that by including the constant $C(Z)$, the final temperature would approach the optimal final steady state temperature; this would not be the case had the algorithm (6-2) been considered, because it is assumed $K(Z)$ is not a function of time. Another advantage of Equation (6-3) is that the control temperature range is decreased and the output of the controller does not have to change rapidly from low range to high range.

For a given set of initial conditions, the constants $C(Z)$ and $K(Z)$ in Equation (6-3) are functions of $Z$. Therefore, a search must be formed to obtain the optimal values of $C(Z)$ and $K(Z)$. Since the spatial coordinate is discretized, only the discrete values of $Z$ could be considered. Initially, the location of the feedback sensor was specified; then a direct search using Powell's method was used to obtain the optimal parameters. The optimal parameters and the corresponding optimal cumulative yield for a single feedback controller as a function of feedback sensor location are tabulated in Table 5.
### TABLE 5

**Optimal Parameters for One Feedback Sensor Controller**

\[ TC(t) = C(Z) + K(Z)CB(t,Z) \]

<table>
<thead>
<tr>
<th>( Z )</th>
<th>( C(Z) )</th>
<th>( K(Z) )</th>
<th>Yield g-mole/liter</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>325.034</td>
<td>-12.64</td>
<td>12.922</td>
</tr>
<tr>
<td>0.10</td>
<td>498.875</td>
<td>-1582.52</td>
<td>13.227</td>
</tr>
<tr>
<td>0.15</td>
<td>419.569</td>
<td>-660.91</td>
<td>13.22212</td>
</tr>
<tr>
<td>0.20</td>
<td>383.681</td>
<td>-330.43</td>
<td>13.2196</td>
</tr>
<tr>
<td>0.25</td>
<td>366.080</td>
<td>-192.76</td>
<td>13.2203</td>
</tr>
<tr>
<td>0.30</td>
<td>355.55</td>
<td>-122.63</td>
<td>13.22218</td>
</tr>
<tr>
<td>0.35</td>
<td>349.597</td>
<td>-86.31</td>
<td>13.22219</td>
</tr>
<tr>
<td>0.40</td>
<td>346.075</td>
<td>-65.867</td>
<td>13.220</td>
</tr>
<tr>
<td>0.60</td>
<td>340.250</td>
<td>-36.27</td>
<td>13.155</td>
</tr>
<tr>
<td>0.80</td>
<td>336.862</td>
<td>-25.12</td>
<td>13.080</td>
</tr>
<tr>
<td>1.00</td>
<td>335.323</td>
<td>-20.27</td>
<td>13.031</td>
</tr>
</tbody>
</table>
OPTIMAL YIELD AFTER STEP DISTURBANCE
ONE FEEDBACK SENSOR (LOCATION z=0.10)
From Table 5 it is seen that the constant and the gain of the feedback controller are a strong function of feedback sensor location. As the sensor is moved further from the feed entrance both \( C(Z) \) and \( K(Z) \) decrease. The optimal feedback sensor location were found to be at \( Z = 0.10 \) with \( C(Z) = 498.875 \) and \( K(Z) = -1582.52 \) which indicates a negative feedback. The cumulative yield using the optimal values of the parameters is 13.227 g-mole/liter. The optimal feedback control and the corresponding optimal instantaneous yield are plotted in Figures 6-1 and 6-2. The optimal control initially drops to \( TC = 280^\circ K \), then it starts oscillating about the final steady state control, \( TC = 325.4 \). The amplitude of the oscillations decreases as time increases and finally the control reaches its final steady state value.

Comparing the optimal feedforward and feedback control, Figures 5-4 and 6-1, it is seen that the initial drop in the control for the feedforward control is not as much as that of the feedback control and the initial oscillations are absent. However, for any time subsequent to one residence time, \( t = 10 \) min., the oscillations in the feedback control are absent and the control reaches the steady state control in a time less than the final time. In contrast, the feedforward control does not reach the steady state value before the specified final time. The decrease in the cumulative yield using the feedback control could be explained by comparing the instantaneous yield with the optimal feedforward yield, Figures 6-2 and 5-5. The reduction in the total yield is caused by the presence of the sharp oscillations in the instantaneous yield of feedback control after one residence time.
OPTIMAL CONTROL AFTER STEP DISTURBANCE
ONE FEEDBACK SENSOR (LOCATION Z=10.35)

FIGURE 6-3
OPTIMAL YIELD AFTER STEP DISTURBANCE
ONE FEEDBACK SENSOR (LOCATION Z = 0.35)

FIGURE 6-4
Next to the optimal controller, from Table 5, is a controller with feedback sensor at $Z = 0.35$, $C(Z) = 349.60$, and $K(Z) = -86.31$. The gain for this controller is much smaller than the gain for the optimal controller. The cumulative yield using these parameters is 13.222 g.mole/liter which is not far from the yield using the best feedback control. The control and the corresponding instantaneous yield are plotted in Figures 6-3 and 6-4. Comparing these figures with Figures 6-1 and 6-2 it is seen that the sharp oscillations are absent, but the control does not approach the steady state control before the final time, $t_f = 25$ min. In view of the response of the controller it is recommended that for the feedback sensor location be located at $Z = 0.35$.

D. Multiple Feedback Sensors

One of the distinct properties of the distributed parameter systems is that multiple feedback sensors can be used to achieve the control. In contrast to the single sensor, finding the sensors locations for the multiple sensor feedback controller is much more difficult, because it involves searching for two or more parameters depending on the number of sensors. Another problem is associated with the fact that the system is discretized and the variables are measured at discrete points; therefore, the developed search techniques are not applicable in the determination of the optimal sensors locations and the optimal controller parameters simultaneously.

The following algorithm for a two feedback sensors controller was selected

$$TC(t) = C(Z) - K_1(Z_1)CB(t,Z_1) - K_2(Z_2)CB(t,Z_2)$$  \hspace{1cm} (6-4)
where

\[ C(Z) = \text{The constant of the controller} \]
\[ K_1(Z_1) = \text{gain of the first sensor} \]
\[ K_2(Z_1) = \text{gain of the second sensor} \]
\[ Z_1 \text{ and } Z_2 = \text{location of the first and the second feedback sensors respectively} \]

To obtain the optimal parameters locations of the feedback sensors were assumed and Powell's method was used to obtain the optimal parameters for the particular choice of sensor locations. This process was repeated and the results of each run was compared to the previous one. The optimal locations were found to be \( Z_1 = 0.30 \) and \( Z_2 = 0.55 \); the optimal parameters corresponding to these locations were found to be

\[ C = 355.68 \quad K_1 = 89.70 \quad K_2 = 19.71 \]

Using this optimal two feedback sensor controller the optimal cumulative yield was found to be 13.238 g.mole/liter. The control and the corresponding instantaneous yield, using the optimal two feedback sensors controller, are plotted in Figures 6-5 and 6-6 respectively. Comparing these figures to Figures 6-1 and 6-2 for one feedback sensor, it is seen the oscillatory behavior is absent and the control curve is smoother. The instantaneous yield is quite similar to the optimal yield Figure 5-5. Therefore, addition of a new feedback sensor has resulted in a higher yield and a smoother control function.

A three feedback sensor controller was also used. The following controller algorithm was assumed.
Optimal control after step disturbance
Two feedback sensors

Figure 6-5

Time (min.)

Control TC (T) (°K)
OPTIMAL YIELD AFTER STEP DISTURBANCE
TWO FEEDBACK SENSORS

FIGURE 6-6
where
\[ K_3(Z_3) = \text{the gain of the third feedback sensor} \]
\[ Z_3 = \text{the location of the third feedback sensor.} \]

The same technique as for the two feedback controller was used to obtain the optimal feedback sensors locations. The procedure was more difficult than the previous cases, because it involved three-parameters. The result was
\[ Z_1 = 0.25 \quad Z_2 = 0.5 \quad Z_3 = 0.75 \]

Using the optimal locations the optimal parameters were calculated to be
\[ C = 362.84, \quad K_1(Z_1) = 122.79, \quad K_2(Z_2) = 22.22, \]
\[ K_3(Z_3) = 5.79 \]

The optimal cumulative yield using the optimal controller was found to be 13.243 g.mole/liter which is higher than the yield obtained by using a two feedback sensors controller. The control and corresponding instantaneous yield are plotted in Figures 6-7 and 6-8. The control function is smoother than the one obtained by a two feedback controller. The cumulative yield is almost equal to the yield using feedforward control; this may be observed from comparison of the instantaneous yield plots, Figures 5-5 and 6-8, which are quite similar.
OPTIMAL YIELD AFTER STEP DISTURBANCE
THREE FEEDBACK SENSORS

FIGURE 6-8

YIELD, G-MOLE/LITER
0.52
0.48
0.44
0.40

TIME (MIN.)
0.00 5.00 10.00 15.00 20.00 25.00
E. Feedback vs. Feedforward Control

The results of this chapter show that the design of feedback control for distributed parameter systems is quite feasible and practical. As it was seen the optimal feedback controllers were obtained for one set of initial conditions. To obtain a realistic solution, which is applicable to any feed conditions, a wide range of initial conditions must be investigated. Then a table may be constructed which gives the locations and the parameters of the controllers. For intermediate feed conditions, extrapolation of the parameters may be necessary.

Table 6 gives the optimal cumulative yield for the feedforward and different feedback controllers.

<table>
<thead>
<tr>
<th>Type of Controller</th>
<th>Cumulative Yield g-mole/liter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feedforward</td>
<td>13.246</td>
</tr>
<tr>
<td>Feedback (one sensor)</td>
<td>13.227</td>
</tr>
<tr>
<td>Feedback (two sensors)</td>
<td>13.238</td>
</tr>
<tr>
<td>Feedback (three sensors)</td>
<td>13.243</td>
</tr>
</tbody>
</table>

Here it is seen that using the maximum principle for distributed parameter systems (feedforward control) results in the highest cumulative yield. The yield using feedback controllers depends on the number of feedback sensors; as the number of feedback sensors are increased the cumulative yield is also increased. A three feedback sensors results in yield approximately equal to that of feedforward control.
The number of feedback sensors should be determined from an economical standpoint. If the increase in the yield justifies the additional feedback sensors, then more may be used. In this specific case, one feedback sensor at the optimal location is probably sufficient.

The main advantage of feedback controller over the feedforward control is that it takes corrective action for further disturbance in the system. Obtaining the feedback control of the system was much simpler than calculating the feedforward control. The only problem associated with the feedback controller was the determination of the optimal sensor locations, which increased in complexity as the number of feedback sensors are increased.
State of the art optimal control theory for the distributed parameter system was applied to a plug-flow tubular reactor in which a consecutive chemical reaction was occurring. The control of the reactor was achieved by the manipulation of the cooling water temperature. A gradient technique was used to obtain the optimal control. For a step change in the feed conditions, it was shown the application of the optimal control would result in a higher yield than the instantaneous application of the final optimal steady state control.

Upon linearization of the systems mathematical model, the frequency response was obtained by a method due to Sinai and Foss (68). Then, the frequency response was used to find the overall transfer function of the system. The minimum principle for lumped parameter systems was applied to the approximate system (resulting from the transfer functions) in order to obtain an sub-optimal control. This sub-optimal control was shown to result in a yield higher than the yield using the new steady state optimal control, but slightly lower than the yield obtained using the optimal control.

These results indicated that:

1. The application of optimal control theory for distributed parameter systems involves sufficient mathematical and computational complications as to make it difficult, if not impossible, to implement the theory on systems of practical importance in the chemical process industries. This is particularly true if it is desired to obtain the
control faster than real time so that it may be applied on line by a digital control computer.

The control action obtained by considering the system's approximate transfer function results in a control that is much easier to determine and implement. Since only a small loss in yield from the theoretical optimal results, it would appear that this method shows considerable promise for future application in the process industries.

A search technique was used to obtain optimal feedback control of the system. It was observed that the yield was a function of number of feedback sensors and their locations. The cumulative yield improved as the number of feedback sensors was increased. Using three feedback sensors resulted in a cumulative yield approximately equal to that of the optimal feedforward control.

This method also shows considerable promise since it indicates that a small number of feedback sensors are all that are required to obtain a yield essentially equivalent to the optimal yield. Considerable work remains to be done to determine for what systems and under what operating conditions similar results might be achieved.
NOMENCLATURE

A  dimensionless constant defined as \( \frac{R_{c_1}}{R_{c_0}} \)

\( b_1 \)  \( \frac{(-\Delta H_A)}{C_p \rho} \)

B  dimensionless constant defined as \( \frac{R_{c_2}}{R_{c_0}} \)

\( b_2 \)  \( \frac{(-\Delta H_B)}{C_p \rho} \)

C(S)  Laplace transform of the output variable

C  cooling water temperature for feedback controller

\( C_1, C_2, C_3 \ldots \)  boundary conditions for the state variables

\( C_p \)  heat capacity of the reacting fluid

CA, CB  concentration of reactant A and product B in the reactor

\( CA_i, CB_i, T_i \)  imaginary parts of complex variables \( \overline{CA}, \overline{CB}, \overline{T} \)

\( CA_0, CB_0 \)  concentrations of A and B in the feed

\( CAR, CBR, TR \)  real parts of complex variables \( \overline{CA}, \overline{CB}, \overline{T} \)

\( d_A, d_B, d_T \)  boundary conditions on the reactor

\( E_1, E_2 \)  activation energies

\( \tilde{F} \)  vector valued functions, \( \tilde{F}_1, \tilde{F}_2, \ldots, \tilde{F}_n \)

\( G, G_1, G_2 \)  transfer functions

\( g_1 \)  forcing function

\( g_2 \)  control function

GH  upper limit of \( g_2 \)

GL  lower limit of \( g_2 \)

GN  steady state gain of the system

H  Hamiltonian function

\( \tilde{H}, \tilde{H} \)  integrated H with respect to Z and t

\( \Delta H_A, \Delta H_B \)  heat of reactions
I  increments along the reactor length  
\( i \)  \( \sqrt{-1} \)  
\( J \)  cost function  
\( K_1, K_2 \)  reaction rate constants  
\( K_1, K_2, K_3 \)  feedback gains  
\( K_{10}, K_{20} \)  frequency factors for the rate constants  
\( L \)  reactor length  
\( M \)  input to the system  
\( n \)  increments along the time axis  
\( \bar{P} \)  adjoint variables, \( (P_1, P_2 \ldots) \)  
\( R \)  gas constant  
\( r \)  reactor diameter  
\( S \)  Laplace domain variable  
\( T \)  temperature of the reacting fluid in the reactor  
\( T^* \)  dimensionless temperature defined as \( \frac{T_0}{\Delta T} \)  
\( t \)  time variable  
\( t_o \)  initial time  
\( t_f \)  final time  
\( TC \)  cooling water temperature (control)  
\( TO \)  feed temperature  
\( \bar{U} \)  control vector \( (U_1, U_2 \ldots) \)  
\( \Delta\bar{U} \)  change in the control vector  
\( u \)  overall heat transfer coefficient  
\( v \)  feed rate  
\( \bar{X} \)  state variables \( (X_1, X_2, \ldots) \)  
\( XKP \)  1-steady state gain
\( X_0 \) initial conditions on the state variables

\( Z \) distance variables

\( Z_1, Z_2, Z_3 \) locations of feedback sensors

\textbf{Greek}

\( \alpha \) heat exchange parameter, \( \frac{2u}{v \cdot C_p \cdot \rho} \)

\( \Delta \) increment

\( \delta \) first-order variation

\( \epsilon_j \) step size of iteration

\( \Delta \epsilon_p \) change in the step size of iteration

\( \Lambda \) function defined in Equation (2-17)

\( \theta \) scalar function

\( \pi \) 3.14159

\( \rho \) density of the reacting fluid

\( \tau_0 \) dead time

\( \tau_1, \tau_2 \) time constants

\( \varphi \) scalar function

\( \Omega_A, \Omega_B, \Omega_T, \Omega_{TB} \) sensitivity functions

\( \omega \) a set defining the constraints on the control

\( \omega \) angular velocity

\textbf{Subscripts:}

\( i \) length index

\( n \) time index

\( ss \) steady state values

\textbf{Superscripts:}

\( T \) transpose
* optimal values

~ dimensionless variables

perturbation from the steady state

complex variables

Symbol:

< , > inner product.


55. Planchard, J. A., Personal Communication, Louisiana State
University, Baton Rouge, 1970.


APPENDIX A

DERIVATION OF THE SYSTEMS EQUATIONS
System:

A tubular reactor of length L, feed rate of \( V \) ft\(^3\)/hr., concentration of feed \( \text{CAO} \) \( \frac{1 \text{ lb-mole}}{3 \text{ ft}} \), and \( \text{CBO} \) \( \frac{1 \text{ lb-moles}}{3 \text{ ft}} \).

Reaction:

\[
\frac{K_1}{A} \quad \frac{K_2}{B} \quad C
\]

Rate of Production of A:

\[
\dot{r}_A = -K_1CA
\]  

(A-1)

Rate of Production of B:

\[
\dot{r}_B = K_1CA - K_2CB
\]  

(A-2)

Material balance on A and B in reactor length

\[
\text{Input-Output} = \text{Accumulation}
\]

\[
\frac{\partial CA}{\partial t} = -K_1CA(t,Z) - V \frac{\partial CA(t,Z)}{\partial Z}
\]  

(A-3)

\[
\frac{\partial CB}{\partial t} = K_1CA(t,Z) - K_2CB(t,Z) - V \frac{\partial CB(t,Z)}{\partial Z}
\]  

(A-4)

Energy Balance on length \( \Delta Z \) of reactor

\[
\text{Input-Output} = \text{Accumulation}
\]

\[
(\pi r^2 \Delta Z)(-\Delta HA)K_1CA(t,Z) + (\pi r^2 \Delta Z)(-\Delta HB)K_2CB(t,Z)
\]

\[
+ (2\pi r \Delta Z)(u)[TC(t)-T(t,Z)] - (\pi r^2 \Delta Z)\rho CpV \frac{\partial T}{\partial Z}
\]

\[
= (\pi r^2 \Delta Z)(\rho Cp) \frac{\partial T}{\partial t}
\]  

(A-5)

Divide by \( \pi r^2 \rho Cp \) to get:

\[
\frac{\partial T}{\partial t} = \left( \frac{\Delta HA}{\rho Cp} \right)K_1CA(t,Z) + \left( - \frac{\Delta HB}{\rho Cp} \right)K_2CB(t,Z)
\]

\[
+ \frac{2u}{r \rho Cp} [TC(t)-T(t,Z)] - V \frac{\partial T}{\partial Z}
\]  

(A-6)
Define
\[ a = \frac{\Delta H_A}{\rho C_p} \quad b = \left( -\frac{\Delta H_B}{\rho C_p} \right) \quad \alpha = \frac{2u}{r \rho C_p} \]

Substitute in Equation (A-6) to obtain:

\[ \frac{\partial T(t, z)}{\partial t} = a K_1 C_A(t, z) + b K_2 C_B(t, z) + \alpha [T_C(t) - T(t, z)] \]

\[- v \frac{\partial T(t, z)}{\partial z} \] (A-7)
APPENDIX B

SOURCE PROGRAM FOR OPTIMAL STEADY STATE SOLUTION
THIS PROGRAM OBTAINS THE OPTIMAL STEADY STATE COOLING WATER TEMPERATURE USING THE PATTERN SEARCH TECHNIQUE.

DIMENSION P(3), STEP(3)

ESTIMATE THE INITIAL VALUE OF THE PARAMETER AND THE INITIAL STEP SIZE

P(1) = 320.
STEP(1) = 10.

START THE PATTERN SEARCH

CALL PATTERN(1, P, STEP, 4, 1, CAST)
STOP
END
SUBROUTINE PROG(P,CKST)

THIS SUBROUTINE COMPUTES THE EXIT CONCENTRATION FOR A GIVEN STEADY STATE COOLING WATER TEMPERATURE

DIMENSION P(3)
F1(CA,T)=-A1*CA/EXP(9000./T)
F2(CA,CA,CH,T)=A1*CA/EXP(9000./T)-B1*CH/EXP(15000./T)
F3(CA,CA,CH,T)=AP*CA/EXP(9000./T)+BP*CB/EXP(15000./T)+10**(TCST-T)
1 /3.0
DATA A1,B1,AP,BP,E1,E2,V,AL,BH,DZ,ALP/5.35E11,4.61E18,5.35E13,
1 =-2.305E20,9000.,15000.,0.,10.,100.,=50.,0.05,0.333333/;
DELT=0.05

READ THE INITIAL FEED CONDITIONS,
SOLVE THE STEADY STATE EQUATIONS TO OBTAIN THE BOUNDARY CONDITIONS ON
THE STATE VARIABLES,
TCST=P(1)

CA=0.95
CH=0.05
T=331.4
DB 2 I=1,20
AK1=DELT*F1(CA,T)
AP1=DELT*F2(CA,CH,T)
AQ1=DELT*F3(CA,CH,T)
AK2=DELT*F1(CA+AK1/2.,T+AQ1/2.)
AP2=DELT*F2(CA+AK1/2.,CB+AP1/2.,T+AQ1/2.)
AQ2=DELT*F3(CA+AK1/2.,CB+AP1/2.,T+AQ1/2.)
AK3=DELT*F1(CA+AK2/2.,T+AQ2/2.)
AP3=DELT*F2(CA+AK2/2.,CB+AP2/2.,T+AQ2/2.)
SUBROUTINE PATTERN(NP,P,STEP,NR0,INH,COST)

THIS SUBROUTINE USES THE PATTERN SEARCH

DIMENSION P(NP),STEP(NP),R1(1000),R2(1000),T(1000),S(1000)

C-----STARTING POINT

L=1
ICK=2
ITTER=0
D05 I=1,NP
81(I)=P(I)
B2(I)=P(I)
T(I)=P(I)
S(I)=STEP(I)*10.

C-----INITIAL BOUNDARY CHECK AND COST EVALUATION

CALL BOUNDS(P,IBUT)

IF(IBUT.LE.0)G8T810

IF(IBUT.LE.0)G8T86
WRITE(6,1005)
WRITE(6,1000)(J,P(J),J=1,NP)

C-----BEGINNING OF PATTERN SEARCH STRATEGY

D099 INRD=1,NRD

D012 I=1,NP

S(I)=S(I)/10.

IF(1.I.EQ.0)G8T920
WRITE(6,1003)
WRITE(6,1000)(J,S(J),J=1,NP)
20  IFAIL=0
C-----PERTURBATION ABOUT T
5830  I=1,NP
   IC=0
21  P(I)=T(I)+S(I)
   IC=IC+1
   CALL BOUNDS(P,I9UT)
   IF(J8UT.GT.0)G08T023
   CALL PR8C(P,C2)
      L=L+1
   IF(IS.LT.3)G08T022
   WRITE(6,1002)L,C2
   WRITE(6,1000)(J,P(J),J=1,NP)
22  IF(C1.C2)23,23,25
23  IF(IC.GE.2)G08T024
   S(I)=S(I)
   G08T021
24  IFAIL=IFAIL+1
   P(I)=T(I)
   G08T030
25  T(I)=P(I)
   C1=C2
   CONTINUE
   IF(IFAIL.LT.NP)G08T035
   IF(ICK.EQ.2)G08T090
   IF(ICK.EQ.1)G08T035
   CALL PR8C(T,C2)
      L=L+1
   IF(IS.LT.2)G08T031
   WRITE(6,1002)L,C2
   WRITE(6,1000)(J,T(J),J=1,NP)
31  IF(C1.C2)32,34,34
32  ICK=1
5833  I=1,NP
C1 = C2
35

B1 = 0
D839 I = 1, NP
B2(I) = T(I)
IF (ABS(B1(I)-B2(I)) * LT 1.0F-20) IB1 = IB1 + 1
39

CONTINUE
IF (IB1 EQ NP) G8T890
ICK = 0
ITER = ITER + 1
IF (IB LT 2) G8T840
WRITE (6, 1001) ITER, C1
WRITE (6, 1000) (J, T(J), J = 1, NP)

C == ACCELERATION STEP
40

SJ = 1.0
D845 I = 1, NP
D842 I = 1, NP
42

PI = T(I)
SJ = SJ * 1
CALL BOUNDS(T, I8UT)
IF (I8UT LT 1) G8T846
IF (II EQ 11) ICK = 1
45

CONTINUE
46
D847 I = 1, NP
47
B1(I) = B2(I)
G8T820
90
D891 I = 1, NP
91
T(I) = B2(I)
99
CONTINUE
D8190 I = 1, NP
100    P(I)=T(I)
       COST=C1
       IF(IP.LT.6)RETURN
       WRITE(6,1004)(C1)
       WRITE(6,1000)(J,P(J),J=1,NP)
       RETURN
1000   FORMAT(10X,5(I7,E13.6)/*)
1001   FORMAT(/1X14HITERATION NO.,15/5X,5HCBST=,E15.6,20X,10HPARAMETERS)
1002   FORMAT(10X3HNO.,I4,8X5HCBST=F15.6)
1003   FORMAT(/1X28HSTEP SIZE FOR EACH PARAMETER )
1004   FORMAT(1H113HANSWERS AFTER,13,2X,23HFUNCTIONAL EVALUATIONS //
           5X5HCBST=E15.6,20X,18HOPTIMAL PARAMETERS )
1005   FORMAT(1H135HINITIAL PARAMETERS OUT OF BOUNDS )
       RETURN
       END
APPENDIX C

SOURCE PROGRAM FOR OPTIMAL
FEEDFORWARD SOLUTION
* THIS PROGRAM DETERMINES THE OPTIMAL COOLING WATER TEMPERATURE FOR *
* THE JACKETED TUBULAR REACTOR AFTER STEP CHANGE IN THE FEED CONDITIONS.*
* THE GRADIENT TECHNIQUE IS USED.*

NOMENCLATURE

A1.....FREQUENCY FACTOR
B1.....FREQUENCY FACTOR
E1.....ACTIVATION ENERGY
E2.....ACTIVATION ENERGY
AH.....HEAT OF REACTION
RH.....HEAT OF REACTION
ALP.....REACTOR PARAMETER
V.....FEED FLOW
TCST.....STEADY STATE CONTROL
EPS.....PROPORTIONALITY CONSTANT
DZ.....Z INCREMENT
DT.....TIME INCREMENT
DELZ.....Z INCREMENT
KDTP.....PRINTING INTERVAL
NIT.....ITERATION NO.

COMMON CAP,CBP,TTP,A1,B1,AH,BH,E1,F2,DT,XX1,XX2,XX3,XX1T,XX2T,XX1N,XX2N,
1 BXK2,EX1,EX2,C1,C2,C3,C4,C5,C6,C1B,C2B,C3B,C4B,C5B,C6B,
2 ALT,XL1,XL2,XL3,XL1N,XL2N,DL,BV,AMV,V,DZ

DIMENSION CAT(21),CBT(21),CTT(21),CAN(21),CBN(21),TN(21),CAS(21,51)
1 ,CBS(21,51),TTS(21,51),XL1(21),XL2(21),XL3(21),XL1N(21),XL2N(21)
2 ,XL3N(21),ACT(21),ACT(21),TCT(21),TC(51),XS(51,21),A(3,4),X(3)
3 \( i'(3, 3), TC6(i1) \)
\[ F1(CA, T) = A1 * CA / \exp(9000^\circ / T) \]
\[ F2(CA, CB, T) = A1 * CA / \exp(9000^\circ / T) * B1 * CB / \exp(15000^\circ / T) \]
\[ F3(CA, CB, T) = A1 * CA / \exp(9000^\circ / T) * B1 * CB / \exp(15000^\circ / T) + 10 * (TCST = T) \]
1 /3 0
\[ A1 = 5.35E11 \]
\[ B1 = 4.61E11 \]
\[ AP = 100 * A1 \]
\[ BP = 50 * B1 \]
\[ E1 = 9000^\circ \]
\[ E2 = 15000^\circ \]
\[ V = 0.10 \]
\[ AH = 100^\circ \]
\[ BH = 50^\circ \]
\[ DZ = 0.05 \]
\[ ALP = 1 / 3.0 \]
\[ TCST = 316.4 \]
\[ EPS = 190^\circ \]
\[ KDP = 5 \]
\[ KTP = 0 \]

GUESS THE OPTIMAL CONTROL FOR THE FIRST ITERATION

DB 44 I = 1, 50
\[ TC(T) = 325.4 \]
\[ TC6(I) = TC(I) \]
44 CONTINUE
\[ VEPS = 1 \]
DB 14 NIT = 1, 25
\[ EPS = VEPS + 10^\circ \]
\[ IF(NIT < KTP) = 8, 97, = 7 \]
97 WRITE (6, 78); II
READ THE INITIAL FEED CONDITIONS.
SOLVE THE STEADY STATE EQUATIONS TO OBTAIN THE BOUNDARY CONDITIONS ON
THE STATE VARIABLES.

CA=0.95
CB=0.05
T=331.4
DO 2 I=1,20
AK1=DELZ*F1(CA,T)
AP1=DELZ*F2(CA,CB,T)
AQ1=DELZ*F3(CA,CB,T)
AK2=DELZ*F1(CA+AK1/2.,T+AQ1/2.)
AP2=DELZ*F2(CA+AK1/2.,CB+AP1/2.,T+AQ1/2.)
AQ2=DELZ*F3(CA+AK1/2.,CB+AP1/2.,T+AQ1/2.)
AK3=DELZ*F1(CA+AK2/2.,T+AQ2/2.)
AP3=DELZ*F2(CA+AK2/2.,CB+AP2/2.,T+AQ2/2.)
AQ3=DELZ*F3(CA+AK2/2.,CB+AP2/2.,T+AQ2/2.)
AK4=DELZ*F1(CA+AK3,T+AQ3)
AP4=DELZ*F2(CA+AK3,CB+AP3,T+AQ3)
AQ4=DELZ*F3(CA+AK3,CB+AP3,T+AQ3)
CA=CA+(AK1+2.*AK2+2.*AK3+AK4)/6.
CB=CB+(AP1+2.*AP2+2.*AP3+AP4)/6.
T=T+(AQ1+2.*AQ2+2.*AQ3+AQ4)/6.

STORE THE BOUNDARY CONDITIONS
C
CAT(I)=CA
CBT(I)=CB
TT(I)=T
ACT(I)=CAT(I)
BCT(I)=CBT(I)
TCT(I)=TT(I)
2 CONTINUE

READ IN THE NEW FEED CONDITIONS

CAS=0.65
CBS=0.05
T0=331.4
DT=10.*DZ
ALT=ALP+DT/2.
VTZ=V*DT/DZ
AMV=1.*VTZ
APV=1.*VTZ
TM=0.
KTP=0

SOLVE THE STATE EQUATIONS FORWARD IN TIME AND STORE THE STATE VARIABLES
AT EACH GRID POINT

DB 9 N=1,50
TM=TM+DT
60 DO 80 I=1,20
CAN(I)=CAT(I)
CBSN(I)=CBT(I)
80 T\N(I)=TT(I)
IF(K-4)31,15,16
16 CONTINUE
DO 70 I=1,20
CAS(I,N)=CAT(I)
CBS(I,N)=CHT(I)
70 TTS(I,N)=TT(I)
IF(NEPS*ER+1)69 T9 91
IF(NIT*KTPR)9,91,91
91 IF(KTP=4)54,54,9
54 WRITE(6,21)TM,CBS(20,N),TC(N)
KTP=KTP+KDTP
9 CONTINUE

READ IN THE FINAL VALUES OF THE ADJOINT VARIABLES

XL18=0.
XL28=1.0/V
XL38=0.0
NB=0

START INTEGRATING THE SYSTEM OF THE ADJOINT EQUATIONS BACKWARD IN TIME

DB 90 NB=1.50
TM=TM-DT
N=51-NB
IF(N=1)73,73,74
73 CAP=(CAS(20,N)+CAS(19,N)+ACT(19)+ACT(20))/4.*
CSP=(CBS(20,N)+CBS(19,N)+BCT(19)+BCT(20))/4.*
TTP=(TTS(20,N)+TTS(19,N)+TCT(20)+TCT(19))/4.*
G9 TO 75
CALL THE MATRIX OF COEFFICIENTS

CALL COEF

USE THE GAUSSIAN ELIMINATION TO SOLVE THE SYSTEM OF THREE LINEAR EQUATIONS IN THREE UNKNOWNS

CALL SOLVE(A,X)
XL1(1)=X(1)
XL2(1)=X(2)
XL3(1)=X(3)
DO 62 J=2,20
I=21-J
IF(N.EQ.1)GO T9 99
IF(I.EQ.1,41,41,42
41 CAP=(2*CAS+CAS(1,N)+CAS(1,N-1))/4.
CBP=(2*CBS+CBS(1,N)+CBS(1,N-1))/4.
TTP=(2*TTS(1,N)+TTS(1,N-1))/4.
GO TO 43
42 CAP=(CAS(I,N)+CAS(I-1,N)+CAS(I,N-1)+CAS(I-1,N-1))/4.
CBP=(CBS(I,N)+CBS(I-1,N)+CBS(I,N-1)+CBS(I-1,N-1))/4.
TTP=(TTS(I,N)+TTS(I-1,N)+TTS(I,N-1)+TTS(I-1,N-1))/4.
GO TO 43
99 IF(I.EQ.1)98,93,88
98 CAP=(2*CAS+CAS(1,N)+ACT(1))/4.
CBP=(2*CBS+CBS(1,N)+ACT(1))/4.
TTP=(2*TTS(1,N)+TCT(1))/4.
CALCULATE THE CUMULATIVE YIELD OF B

CBL=0
DO 55 I=2,49
55 CBL=CBL+CBS(20,I)
Y=DT/2*(CBS(20,1)+2*CBL+CBS(20,50))
IF(NEPS.EQ.1)GO TO 79
IF(NIT.EQ.KTPR)96,79,79
79 WRITE(6,56)Y
NEPS=0
KTPR=KTPR+KTP

COMPARE THE NEW YIELD TO THE YIELD FROM THE PREVIOUS ITERATION
C
26 IF(Y.LE.YR) GO TO 25
YR=Y
GO TO 32
C
C
C
C

IF THE NEXT YIELD IS LESS THAN THE PREVIOUS YIELD DECREASE THE
PROPORTIONALITY CONSTANT

35 EPS=EPS*20.
NEPS=1
32 DB 51 KN=1/50
N=51-KN
TM=TM+DT
SUMEV=0.
SUMD=0.
DB 52 I=1,19,2
52 SUMEV=SUMEV+X3S(N,I)
DB 53 I=2,18,2
53 SUMD=SUMD+X3S(N,I)
PLA3=DZ/3.*(X3S(N,20)+4.*SUMEV+2.*SUMD+XL39)

DETERMINE THE NEW CONTROL FOR THE NEXT ITERATION

58 TC(KN)=TC8(KN)+EPS*PLA3
51 CONTINUE
   IF(NEPS.EQ.1) GO TO 97
39 37 L=1,50
37 TC8(L)=TC(L)
NEPS=0
14 CONTINUE
48 WRITE(6,68) NIT, Y
    WRITE(6,205)(TC(N), CSP(20,N), N=1,30)
20 FORMAT(1H,8X,'TIME',10X,'CB(1)',9X,'TC(T)''//')
21 FORMAT(7X,F6.2,5X,E12.5,5X,F7.2)
56 FORMAT(/9X,'YIELD' = F10.7/)
68 FORMAT(/9X,'ITERATION NO.' = I2/9X,'OPTIMAL YIELD' = F10.7/)
200 FORMAT(/5X,'PROPORTIONALITY CONSTANT = ',F5.1//)
205 FORMAT(10X,2(2X,F10.5))
STOP
END
SUBROUTINE USES THE STORED VALUES OF THE STATE VARIABLES TO CALCULATE THE COEFFICIENTS FOR THE SYSTEM OF THE ADJOINT EQUATIONS.

DIMENSION A(3,4)

1 COMM8N CAP, CBP, TTP, A1, B1, AH, BH, E1, E2, DT, XK1, XK2, XK1T, XK2T, AXK1, NB,

2 ALT, A, XL1, XL2, XL3, XL1N, XL2N, XL3N, APV, AMV, V, DZ

75 XK1=A1/(10**EXP(9000./TTP))
XK2=B1/(10**EXP(15000./TTP))
XK1T=A1*K2/2.
AXK1=AH*AXK1T
EXK1=E1*EXK1T
EXK2=E2*EXK2T
C1=APV*AXK1T
C2=AMV*AXK1T
C3=APV*AXK1T
C4=AMV*AXK1T
C5=EXK1T*CAP/(AH*TTP**2)
C6=C5*A1
C1B=APV*AXK1T
C2B=AMV*AXK1T
C3B=APV*AXK1T
C4B=AMV*AXK1T
C5B=EXK2T*CBP/(B4*TTP**2)
C6B=C5B*B4
A(1,1)=C1
A(1,2)=X1T
A(1,3) = A(i)1
A(2,1) = v
A(2,2) = c1
A(2,3) = 0
A(3,1) = c7
A(3,2) = c5
A(3,3) = \text{APV} = c6\cdot c6B \cdot \text{ALT}
\text{IF}(\text{IB} \cdot \text{GT} \cdot 1) \text{GO} \text{ TO } 2
\text{IF}(\text{J} \cdot \text{GT} \cdot 1) \text{GO} \text{ TO } 3
1 \ A(1,4) = \text{xK1T/V}
A(2,4) = c2
A(3,4) = (c5\cdot c5B)/V
\text{GO} \text{ TO } 4
3 \ A(1,4) = c2\cdot XL2(J-1) + \text{xK1T} \cdot XL2(J-1) + \text{AXK1} \cdot XL3(J-1)
A(2,4) = c2B\cdot XL2(J-1) + 3\cdot XL2(J-1)
A(3,4) = (\text{AMV} + \text{ALT} + c6\cdot c6B) \cdot XL3(J-1) + (c5\cdot c5B) \cdot XL2(J-1) + c5 \cdot XL1(J-1)
\text{GO} \text{ TO } 4
2 \ \text{IF}(\text{J} \cdot \text{GT} \cdot 1) \text{GO} \text{ TO } 5
A(1,4) = c4\cdot XL1N(1) + \text{K1T} \cdot XL2N(1) + \text{AXK1} \cdot XL3N(1) + 2 \cdot \text{XK1T/V}
A(2,4) = c4B\cdot XL2N(1) + 3\cdot XL2N(1) + 2 \cdot \text{XK2/V} + 2 \cdot \text{DT/DZ}
A(3,4) = (\text{AMV} + c6 \cdot c6B \cdot \text{ALT}) \cdot XL3N(1) + (c5B \cdot c5) \cdot XL2N(1) + c5 \cdot XL1N(1)
1 + 2 \cdot (c5 \cdot c5B)/V
\text{GO} \text{ TO } 4
5 \ A(1,4) = c2 \cdot XL1(J-1) + \text{xK1T} \cdot XL2(J-1) + XL2N(J-1) + XL2N(J-1) + c3 \cdot XL1N(J-1)
A(2,4) = c2B \cdot XL2(J-1) + d \cdot XL2(J-1) + XL3N(J-1) + XL3N(J-1)
A(3,4) = (AMV + \text{ALT} + c6 \cdot c6B) \cdot XL3(J-1) = (c5B \cdot c5) \cdot XL2(J-1) + XL2N(J-1) +
1 \cdot XL2N(J-1) + c5 \cdot (XL1(J-1) + XL1N(J-1) + XL2N(J-1)) + (\text{APV} + \text{ALT} + c6 \cdot c6B) 
2 \cdot XL3N(J-1) + (\text{AMV} + \text{ALT} + c5B + c6) \cdot XL3N(J)
4 \ \text{RETURN}
\text{END}
THIS SUBROUTINE USES THE METHOD OF GAUSSIAN ELIMINATION TO SOLVE A SYSTEM
OF THREE LINEAR EQUATIONS IN THREE UNKNOWNS

DIMENSION A(3,4),X(3,3),Y(3)

105 IF(A(1,1))111,106,111

106 KK=1

109 CONTINUE

WRITE(6,110)

FORMAT(19,ONE UNIQUE SOLUTION)

110 IF(A(1,1))111,109,111

112 R(1,J-1)=A(1,J)-A(1,J)*A(I,J)/A(1,1)

113 E(NN,J-1)=A(1,J)/A(1,1)

114 IF(E(1,J))117,115,116

115 GO TO 109

116 GO TO 117
APPENDIX D

SOURCE PROGRAM TO COMPARE
THE LINEAR AND NONLINEAR STATE
EQUATIONS RESPONSE
THIS PROGRAM COMPARES THE TIME DOMAIN RESPONSE OF THE ACTUAL NON-LINEAR SYSTEM OF THE STATE EQUATIONS TO THE RESPONSE OF THE LINEARIZED SYSTEM OF DIMENSION-LESS STATE EQUATIONS FOR A GIVEN CONTROL.

C       COMMON N,I,RA,RR,RT,RTB,CAT,CBT,TT,CAP,CBP,TTP,CAN,CBN,TTN,TC,A
       1  *SA,SB,ST
       DIMENSION CAT(21),CBT(21),TT(21),CAN(21),CBN(21),TN(21),CBS(21,51)
       1  *ACT(21),BTC(21),TCT(21),TC(51)
       DIMENSION CAP(21),CBP(21),TTP(21),RA(21),RB(21),RT(21),RTB(21)
U       X(3),F(3,4),CBL(51),TNT(21)
       F1(CA,T)=1.5*CA/EXP(9000/T)
       F2(CA,CB,T)=1.5*CA/EXP(9000/T)-0.5*CB/EXP(15000/T)
       F3(CA,CB,T)=AP*CA/EXP(9000/T)+BP*CB/EXP(15000/T)+10**((TCST+1)/3)
       1  /3.0
G1(CA,T)=1.5*EXP(U*T/(T+TS)*CA
G2(CA,CB,T)=1.5*EXP(U*T/(T+TS)*CA-1.5*EXP(U*T/(T+TS)*CB
G3(CA,CB,T)=1.5*EXP(U*T/(T+TS)*CA-1.5*EXP(U*T/(T+TS)*CB*B1
       1  +ALP*(T+T)
       DATA A1,B1,AP,BP,E1,E2,VA,BH,BZ,ALP/5,35E11,4.61E18,5.35E13,
       1  -2.305E20,3000,15000,0.1U,100U,50,0.05,0.33333/1
       TCI=316.4
       14 I=1
       Z=0.0
      DELZ=0.05
      TCST=316.4

READ THE INITIAL FEED CONDITIONS.
CA = 1.45
CB = 0.02
T = 314

DE i n t h e C n t r a l

M 39 4 = 1, 50
39 TC(1) = TC(T)
A1 = 4, 61, 1
ALP = 1, 3, 0

SOLVE THE STEADY STATE EQUATIONS TO OBTAIN THE BOUNDARY CONDITIONS ON
THE ST GE VAR-ASSAY

3 AK1 = DELZ * F1 (CA, T)
   AP1 = DELZ * F2 (CA, CB, T)
   AU1 = DELZ * F3 (CA, CB, T)
   AK2 = DELZ * F1 (CA + AK1 / 2, T + AP1 / 2)
   AP2 = DELZ * F2 (CA + AK1 / 2, CB + AP1 / 2, T + AP1 / 2)
   AU2 = DELZ * F3 (CA + AK1 / 2, CB + AP1 / 2, T + AP1 / 2)
   AK3 = DELZ * F1 (CA + AK2 / 2, T + AP2 / 2)
   AP3 = DELZ * F2 (CA + AK2 / 2, CB + AP2 / 2, T + AP2 / 2)
   AU3 = DELZ * F3 (CA + AK2 / 2, CB + AP2 / 2, T + AP2 / 2)
   AK4 = DELZ * F1 (CA + AK3, T + AP3)
   AP4 = DELZ * F2 (CA + AK3, CB + AP3, T + AP3)
   AU4 = DELZ * F3 (CA + AK3, CB + AP3, T + AP3)
   CA = CA + (AK1 / 2 * AK1 / 2 * AK2 / 2 * AK3 + AK4 / 2)
   CB = CB + (AP1 / 2 * AP2 / 2 * AP3 + AP4 / 2)
   T = T + (AU1 / 2 + AU2 / 2 + AU3 / 2 + AU4 / 2)
   Z = Z + DELZ
STORr THE BOUNDARY CONDпITIONS

CAT(I)=CA
CBT(I)=CB
TT(I)=T
ACT(I)=CAT(I)
BCT(I)=CBT(I)
TCT(I)=TT(I)
I=I+1
IF(Z*GE.0.97)GO TO 77
GO TO 3

READ IN THE NEW FEED CONDITIONS

77 READ(5,100)SA,S3,ST,DT
100 FORMAT(3F7.3,11)
WRITE(6,102)SA,S3,ST
102 FORMAT(1H1,3(F7.3/))
CA8=SA
CB8=S3
TB=ST
DT=10.*DZ
ALT=ALP*DT/2.
VTZ=V*DT/DZ
AMV=1.*VTZ
APV=1.*VTZ
TM=0.*

SOLVE THE STATE EQUATIONS FORWARD IN TIME AND STORE THE STATE VARIABLES
AT EACH GRID POINT

DB 2 N=1,50
TM=TM+DT
60 DB 20 I=1,20
   CAN(I)=CAT(I)
   CBH(I)=CBT(I)
80 TN(I)=TT(I)
   DB 13 K=1,6
   CAH=(2**CAH+CAN(I)+CAT(I))/4*
   CBH=(2**CBH+CBN(I)+CBT(I))/4*
   TH=(2**TB+TN(I)+TT(I))/4*
   PAL=9000./TH
   SBN=15000./TH
   IF (PAL*GT*.60) PAL=.60*
   IF (SBN*GT*.60) SBN=.60*
   XK1=A1/(10**EXP(PAL))
   XK2=B1/(10**EXP(SBN))
   CAT(I)=(2**VTZ*CAH+AMV*CAN(I)+P**(XK1*CAH+DT))/APV
   CBT(I)=(2**VTZ*CBH+AMV*CBN(I)+P**(XK1*CAH=XB2*CBH)*DT)/APV
13 TT(I)=(2**VTZ*TB+AMV*TN(I)+P**(XK1*CAH+XB3*XB4) +
   ALP*(TC(N)-TH))/APV

DB 16 I=2,20
   K=0
   CAH=(CAN(I)+CAT(I-1))/2*
   CBH=(CBN(I)+CBT(I-1))/2*
   TH=(TN(I)+TT(I-1))/2*
81 PAL=9000./TH
   SBN=15000./TH
   IF (PAL*GT*.60) PAL=.60*
   IF (SBN*GT*.60) SBN=.60*
   XK1=A1/(10**EXP(PAL))
   XK2=B1/(10**EXP(SBN))
\[
\begin{align*}
\text{CAT}(I) &= (A \cdot V \cdot \text{CAN}(I-1) + A \cdot V \cdot \text{CAN}(I) - 2 \cdot \text{X} \cdot 1 \cdot \text{CAH} \cdot T - A \cdot V \cdot T \cdot \text{AT}) / A \cdot V \\
\text{CBT}(I) &= (A \cdot V \cdot \text{CBN}(I-1) + A \cdot V \cdot \text{CBN}(I) + 2 \cdot (A \cdot V \cdot \text{X} \cdot \text{K} \cdot 1 \cdot \text{CAH} + A \cdot 0 \cdot E \cdot \text{CB}) \cdot T - A \cdot V \cdot \text{CBT}(I-1) / A \cdot V \\
\text{TT}(I) &= (A \cdot V \cdot \text{T}(I-1) + A \cdot V \cdot \text{T}(I) + 2 \cdot \text{DT} \cdot (A \cdot V \cdot \text{X} \cdot \text{K} \cdot 1 \cdot \text{CAH} + A \cdot V \cdot \text{X} \cdot \text{K} \cdot 1 \cdot \text{CB}) \cdot \text{ALP} \cdot A \cdot V / A \cdot V \\
\text{CAH} &= (\text{CAN}(I-1) + \text{CAN}(I) + \text{CAT}(I-1) + \text{CAT}(I)) / 4 \\
\text{CBT} &= (\text{CBN}(I-1) + \text{CBN}(I) + \text{CBT}(I-1) + \text{CBT}(I)) / 4 \\
\text{TH} &= (\text{TN}(I-1) + \text{TN}(I) + \text{TT}(I-1) + \text{TT}(I)) / 4 \\
K &= K + 1 \\
\text{IF}(K = 4) &= 81, 16, 16 \\
16 &= \text{CONTINUE}
\end{align*}
\]

STORE THE DIMENSIONLESS EXIT CONCENTRATION OF THE DESIRED PRODUCT

DO 70 I=1,20
CBS(I,N) = CBT(I) / 0.95
70 CONTINUE
9 CONTINUE

READ IN THE INITIAL CONDITIONS FOR THE STEADY STATE DIMENSIONLESS EQUATIONS

\[
\begin{align*}
T_0 &= 331.4 \\
C_A &= 0.95 \\
X_{KA} &= 535 \\
X_{KH} &= 4.61 \\
C_A &= 1.0 \\
Z &= 0.0 \\
CB &= 0.05/C_A \\
T_D &= (316.4 - T_0) / (100 * C_A) \\
T_S &= T_S / (100 * C_A) \\
\end{align*}
\]
PART II. THE STEADY STATE SOLUTION FOR THE NONDIMENSIONAL EQUATIONS CALCULATED AND THE SPINIVITY COEFFICIENTS
THE SYSTEM OF THREE LINEAR EQUATIONS IN THREE UNKNOWNS:

CALCULATE THE VALUES OF THE EQUATIONS FOR THE LINEARIZED SYSTEM AND SOLVE

19 (C1) = (C1) = (C1) = (C1) = (C1)
20 (C1) = (C1) = (C1) = (C1) = (C1)
21 (C1) = (C1) = (C1) = (C1) = (C1)
22 (C1) = (C1) = (C1) = (C1) = (C1)
23 (C1) = (C1) = (C1) = (C1) = (C1)
THIS SUBROUTINE CALCULATES THE MATRIX OF COEFFICIENTS FOR THE SYSTEM OF LINEARIZED DIMENSIONLESS STATE EQUATIONS, USING THE STORED VALUES OF THE SENSITIVITY COEFFICIENTS AND THE BOUNDARY CONDITIONS.

SUBROUTINE CBFL
COMMON N, I, RA, RB, RT, RTB, CAT, CBT, TT, CAP, CBP, TTP, CAN, CBN, TTN, TC, A, 1, SA, SB, ST
DIMENSION A(3, 4), CAN(21), CBN(21), TTN(21)
1 CAT(21), CBT(21), TT(21), CAP(21), CBP(21), TTP(21)
2 *RA(21), RB(21), RT(21), RTB(21), TC(51)
DATA V, DT, DZ, E1/1, 0, 0.05, 0.05, 0.5/
CA0 = SA/0.95
CB0 = SB/0.95
TT0 = (ST - 331.4) / (950)
ALP = 10 + 30
BRA = RA(I)
BRB = RB(I)
BRT = RT(I)
BRTB = RTB(I)
ARA = RA(I+1)
ARB = RB(I+1)
ART = RT(I+1)
ARTB = RTB(I+1)
APV = V + V*DT/DZ
AMV = V + V*DT/DZ
A1 = APV + BRA*DT/2,
A2 = AMV + BRA*DT/2,
A1*APV + BRA*DT/2,
A2*AMV + BRA*CT/2,
A3*BRB*DT/2.
A4 = AMV \times DT/2
A3 = 2B9 + \times DT/2
A1 = APV + A3
A2 = AV + A3
A1 = APV + A3
A2 = AV + A3
A5 = B5 \times DT/2
A6 = AMV + A4 \times B1 + A5 + ALP \times DT/2
A7 = APV + A4 \times B1 + A5 + ALP \times DT/2
A8 = APV + A4 \times B1 + A5 + ALP \times DT/2
A9 = APV + A4 \times B1 + A5 + ALP \times DT/2
D2 = A5 + A4
C1 = APV + ARA \times DT/2
C2 = AMV + ARA \times DT/2
C1M = APV + ARA \times DT/2
C2M = AMV + ARA \times DT/2
C3 = ARA \times DT/2
C4 = ART \times DT/2
C3B = ARB \times DT/2
C1B = APV + C3B
C2B = AMV + C3B
C1V = APV + C3B
C2V = AMV + C3B
C5 = ARTB \times DT/2
C6 = AMV + C4 + \times B1 + C5 + ALP \times DT/2
C7 = AMV + C4 + \times B1 + C5 + ALP \times DT/2
C8 = APV + C4 + \times B1 + C5 + ALP \times DT/2
C9 = APV + C4 + \times B1 + C5 + ALP \times DT/2
D1 = C5 + C4
A(1, 1) = C1
A(1, 2) = 3
A(1, 3) = C4
A(2, 1) = C3
A(2, 2) = C1
A(2,3)=C1
A(3,1)=C3
A(3,2)=B1*C3
A(3,3)=C8
IF(I*EQ.1)G8 T9 1
IF(I*EQ.1)G8 T9 2
6 A(1,4)=A2*CAP(I-1)-A4*TTT(I-1)+A1*CAN(I-1)-A4*TTN(I-1)+
   1 C2M*CAN(I)+C4*TTN(I)
   2 +2*A4*TT(I)+C4*TT(I+1)
A(2,4)=A3*CAP(I-1)-A2*CBP(I-1)-D2*TTP(I-1)+A3*CAN(I-1)+
   1 A1N*CBN(I-1)-D2*TTN(I-1)+C3*CAN(I)+C2N*CBN(I)-D1*TTN(I)
   2 +2*DB*TT(I)+D1*TT(I+1)
   1 *CBN(I-1)+A9*TTN(I-1)+C3*CAN(I)+B1*C3*B*CBN(I)+C7*TTN(I)
   2 +ALP*DT*TC(N)*2*
   2 =2*((A4+B1*A5)*TT(I)+(C4+B1*C5)*TT(I+1))
G9 T8 4
2 A(1,4)=A2*CA8-A4*TT8-A1M*CA8-A4*TT8+C2M*CAN(I)+C4*TTN(I)
   2 +2*A4*TT(I)+C4*TT(I+1)
A(2,4)=A3*CA8-A2B*CB8-D2*TT8+A3*CA8-A1N*CB8-D2*TT8+C3*CAN(I)
   1 +C2N*CBN(I)-D1*TTN(I)
   2 +2*DB*TT(I)+D1*TT(I+1)
A(3,4)=A3*CA8+B1*A3B*CB8-A6*TTT+A3*CA8+B1*A3B+C3B*A9*TT8+
   1 +C3*CAN(I)+B1*C3B*CBN(I)+C7*TTN(I)+ALP*DT*TC(N)*2*
   2 =2*((A4+B1*A5)*TT(I)+(C4+B1*C5)*TT(I+1))
G9 T8 4
1 IF(I*EQ.1)G8 T9 5
   CAN(I-1)=CAT(I)
   CBN(I-1)=CBT(I)
   TTN(I-1)=TT(I)
   CAN(I)=CAT(I+1)
   CBN(I)=CBT(I+1)
   TTN(I)=TT(I+1)
G9 T8 6
APPENDIX E

SOURCE PROGRAM FOR GENERATING FREQUENCY DATA AND OBTAINING THE SYSTEM'S TRANSFER FUNCTION
START TO CHANGE THE PRECISION

**C**ASE=2

°C**A**=2

**P**=3.1415927

**D**ATA **N**P,**BP**,**EC**,**STP**,**NPP**1 **N**=1.0**.**0.5**.**0.2**.**1**

**D**IM**E**NS**I**ON **P**p(10)

**I**/**A**H**M**/G(100)**T**EL**(100)**

**C**OM**P**N**X**/S**H**A**/I**PR**I**N**T**/**K**0**R**N**/D**EL**X**/T**1**/P**R**1**N**/T**R**A**G**/C**I**S**T**P**3**/

**B**O**U**N**E**L**E**P**R**E**C**I**S**E**4**Z**(8)**2**W**E**M**(6)**S**U**M**(6)**F**E**U**N**(6)**X**X**K**(4)**6**Y**X**T**1**D**E**L**T

**T**EST**P**HASE **A**NGLE **OF** **E**X**I**T **C**ON**C**E**N**T**R**A**T**I**O**N **OF** **A**

**A**M**P**LITUDE **O**F **E**X**I**T **C**ON**C**E**N**T**R**A**T**I**O**N **AT** **A**

**D**I**M**E**N**S**I**O**N**E**SS **R**E**Q**U**I**R**E**D

**N**O**.** **O**F **D**I**F**E**R**E**N**T**I**A**L **E**Q**U**A**T**I**O**N**S

**N**o**M**E**R**C**AL**C**AL**C**A**L**A**T**E

**********************************************************************

**A** **M**ODEL **K****V****C****A**L**U**S**S** IS **A**S**S**E**S**S**E**D** TO **F**I**L**L **T**HE **P**R**E**R**E**R**U**C**Y **R**E**S**P**O**N**SE**.

**S**Y**S**TE**M**. **S**U**B**S**Y**S**T**E**M**E**R**E**S** IS **U**S**E**D** TO **G**E**T** **T**HE **A**P**P**R**O**X**I**M**A**L **P**A**R**A**M**E**T**E**R**S **F**O**R**

**T**H**I**S **P**R**O**G**R**A**M **C**A**L**C**U**L**A**T**E**S **T**HE **P**R**E**R**E**R**U**C**Y **R**E**S**P**O**N**S**E**S **O**F **T**HE **L****I**N**E**A**R**I**Z**E**D

**********************************************************************
INTEGRATE THE SYSTEM OF LINEARIZED ORDINARY DIFFERENTIAL EQUATIONS THROUGHOUT THE LENGTH OF REACTOR

CALL RUNGA (Z, ZNEW, X, SUM, FUN, CASE)
STORE THE EXIT AMPLITUDE RATIO

CBR = ZNEW(3)
CBI = ZNEW(4)
X = (CBR**2 + CBI**2)**0.5
6(KZ) = X

CALCULATE THE ACTUAL PHASE ANGLE AND STORE

RATIO = ABS(CBI/CBR)
ANGLE = ATAN(RATIO)
READ IN THE INITIAL ESTIMATE OF THE PARAMETERS

READ(5,5)(PP(I),I=1,3)
READ(5,5)(EP(I),I=1,3)
WRITE(6,4)
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WRITE(6,4)
THIS SUBROUTINE DEFINES THE SYSTEM OF DIFFERENTIAL EQUATIONS WHICH ARE INTEGRATED BY SUBROUTINE RUNGE

SUBROUTINE DEFIN(Z,FUN,Y,IT,DELT)
DOUBLE PRECISION Z(6),FUN(6),Y,IT,DELT
COMMON/SHAR/IPRINT,KJMT,DELT,Y,T1,TFIN,TLLOGIC,ISTEP,
G1(CA,T)=XK1*EXP(U*T/(T+TS))*CA
G2(CA,CB,T)=XK1*EXP(U*T/(T+TS))*CA+XK2*EXP(B*T/(T+TS))*CB
G3(CA,CB,T) = XK1*EXP(U*T/(T+TS))*CA+XK2*EXP(B*T/(T+TS))*CB*91
1 +ALP*(T0-T)
DIMENSION RA(21),RB(21),RT(21),RTB(21),DIST(21)
DATA E1,E2,T8,CA6,XK0,XK8/9000,15000,3314,95,5.35E10,
1 4.61F17/
DELZ=0.05
CA=1.0
CB=0.05/CA8
B1=(-50/100.)
T=0.
T0=(316.0*T8)/(100.*CA8)
ALP=10./3.
TS=T8/(100.*CA8)
U=E1/T8
3=E2/T8
XK1=XK0*10.+EXP(U)
XK2=XK8*1.+EXP(U)
DELT=5.*C
DO 2 I=1,21
DIST(I)=DELT*(I-1)
RA(I)=XK1*EXP(U*T/(T+TS))
RA(I)=XK2*EXP(R*T/(T+TS))
RT(I)=XK1*U*EXP(U*T/(T+TS))*CA+TS/(T+TS)**2.
DB 1 J=1,6
1 Z(J)=0.0
Y=0.0
ISTEP=100
J(J)=1.0
TC=1.0
GO TO 30
ENTRY DER(Z,FLV)

DEFINE THE INTERMEDIATE VALUES OF THE SENSITIVITY COEFFICIENTS
I*T1/IELT+1
IF(I*GE.21) Go To 7
8 SA=(RA(I+1)-RA(I))+(T1+DIST(I))/2*DST(I+1)=DIST(I))+RA(I)
SB=(RB(I+1)-RB(I))+(T1+DIST(I))/2*DST(I+1)=DIST(I))+RB(I)
ST=(RT(I+1)-RT(I))+(T1+DIST(I))/2*DST(I+1)=DIST(I))+RT(I)
STB=(RTB(I+1)-RTB(I))+(T1+DIST(I))/2*DST(I+1)=DIST(I))+RTB(I)
GO To 9
7 SA=RA(I)
SB=RB(I)
ST=RT(I)
STB=RTB(I)
9 FUN(1)=w*z(2)=SA*Z(1)=ST*Z(5)
FUN(2)=w*z(1)=SA*Z(2)=ST*Z(6)
FUN(3)=SA*Z(1)=SB*Z(3)+w*z(4)+(ST-FTB)*Z(5)
FUN(4)=SA*Z(2)=sb*Z(4)+(ST-FTB)*Z(6)
FUN(5)=SA*Z(1)+31*SB*Z(3)+(ALP-ST-B1*STB)*Z(5)+w*z(6)+ALP*TC
FUN(6)=SA*Z(2)+31*SB*Z(4)+(ALP-ST-B1*STB)*Z(6)+w*z(5)
30 RETURN
ENTRY DERFIN (Z)
TLOGIC=2.
TFIN=1.

CHECK FOR THE STOPPING CONDITIONS

IF(Y*GE.0.97) TFIN=3.
RETURN
END
THIS SUBROUTINE CALCULATES THE FREQUENCY RESPONSE OF THE MODEL AND FOR A GIVEN SET OF PARAMETERS WHICH ARE CALCULATED IN SUBROUTINE P0W, OBTAINS THE COST FUNCTION WHICH MUST BE MINIMIZED.

SUBROUTINE P0W(P,NR,NP)
COMMON/AHM/G(100),TET(100),KJK
COMPLEX A,B,C,E,CMPLX
DIMENSION P(4,10),H(100),PHI(100)
KJK=KJK+1
PI=3.1415927
GAIN=0.65970
XKP=1.0*GAIN
TAU0=P(NR,1)
TAU1=P(NR,2)
TAU2=P(NR,3)
IK=0
W=0.001
11 IF(W.LT.0.009)GO T0 6
   IF(W.LT.0.09)GO T0 7
   IF(W.LT.0.95)GO T0 9
   IF(W.LT.5.0)GO T0 13
   D=0.1
   GO T0 10
6  D=0.001
   GO T0 10
7  D=0.01
   GO T0 10
8  D=0.1
   GO T0 10
13 D=1.0
10 P=P+D

184
J
X^=1+1
X IM = XKP * SIN (T A U *)
A = C * PLX (XIM, XIM)
= C * PLX (1 + T A U 1 * W)
C = C * PLX (1 + 1 * T A U 2 * W)
E = A / (3 * C)
H (IK) = CA B E (E)
R A T I B = A B S (A I M A G (E) / R E A L (E))
A N G L E = A T A N (R A T I B)
I F (A I M A G (E) GT 0 . 0 * A N D * R E A L (E) LT 0 . 0) G O T 2 0
I F (A I M A G (E) * G T 0 . 0 * A N D * R E A L (E) LT 0 . 0) G O T 3 0
I F (A I M A G (E) LT 0 . 0 * A N D * R E A L (E) LT 0 . 0) G O T 4 0
P H I (IK) = A N G L E
G O T 5 0
2 0 P H I (IK) = A N G L E
G O T 5 0
3 0 P H I (IK) = P I - A N G L E
G O T 5 0
4 0 P H I (IK) = A N G L E - P I
5 0 I F ( * LT 5 0 *) G O T 1 1
S U M = 0
D B 6 0 N P 1 , I K
6 0 S U M = S U M + G (N) * 2 * P S (T E T (N) * P H I (N)) + H (N) * 2 * P S (N , N P + 1 ) * S U M
R E T U R N
E N D
SUBROUTINE IDATA(Y,ITIME)
DOUBLE PRECISION Y,NORM,T1,DEL
COMMON/SHARP/PRINT,PRINT,DELTA,Y,T1,TIME,TLTIC,ISTEP,
DATA <1/
IDUMMY=ITIME
PRINT=PRINT+X
RETURN
END
THIS SUBROUTINE USES FOURTH ORDER RUNGE-KUTTA METHOD TO INTEGRATE A
SYSTEM OF N ORDINARY DIFFERENTIAL EQUATIONS

SUBROUTINE RUN3A (Z,ZNEW,XX,SUM,FUN,ICASE)
DOUBLE PRECISION Z(N),ZNEW(N),SUM(N),FUN(N),XX(4,N),Y,T1,DELT
COMMON/SHAR/PRINT,4JUNT,DELT,Y,T1,TFIN,TL6GIC,ISTEP," parents".
REAL MM,NN
DIMENSION CON(4,3),CN1(4),CN2(4)
IF(ICASE.EQ.2) 39 TO 415
NN=2*3.
MM=1*3.
R=NN*(MM-NN)/(1.*MM**2-2.*MM)
G1=MM**4.*NN**2+15.*NN-2.*
G2=6.*MM**NN-4.*MM**NN+3.*
S=(1.-MM)*G1/(2.*MM*(NN-NN)*G2)
TT=(1.-2.*MM)*(1.-MM)*(1.-NN)/(NN*(NN-NN)*G2)
P=1.
CON1(1)=(6.*MM**NN-2.*MM-2.*NN+1.)/(12.*MM**NN)
CON1(2)=(12.*NN-1.)/(12.*MM*(NN-NN)*(1.-MM))
CON1(3)=(2.*MM-1.)/(12.*NN*(MM-NN)*(1.-NN))
CON1(4)=G2/(12.*NN*(1.-MM)*(1.-NN))
GO TO 416

415 CONTINUE
MM=1*2.
NN=1*2.
P=1.
TT=1.+SURT(0.5)
S=0.5/TT
S=1.-TT
CON1(1)=1./6.
CON1(2)=(2.-TT)/3.
CON1(I)=TT/3.
CON1(4)=1./6.
416 CONTINUE
CONZ(1)=0.
CONZ(2)=MM
CONZ(3)=NN
CONZ(4)=1.
DO 490 I=1,4
DO 490 J=1,N
490 XK(I,J)=0.
KK=0
DO 491 K=1,3
KK=KK+1
DO 491 J=KK,3
491 CON(K,J)=0.
CON(2,1)=MM
CON(3,1)=NN+R
CON(3,2)=R
CON(4,1)=P+TT
CON(4,2)=S
CON(4,3)=TT
CALL DERIV(ZNEW,FUN,N)
IPRINT=0
KBUNT=0
CALL IODATA(ZNEW,N,1)
499 CONTINUE
DO 400 I=1,4
DO 451 J=1,N
Z(J)=ZNEW(J)
DO 451 K=1,3
451 Z(J)=Z(J)+XK(K,J)*CON(I,K)
T1=Y+DELT*CON2(I)
465 CALL DER (Z,FUN)
DO 400 J=1,N
400 XK(I,J)=FUN(J)*DELT
    DO 20 J=1,N
    SUM(J)=0*
    DO 410 I=1,N
    410 SUM(J)=SUM(J)+XK(I,J)*C0N1(I)
420 ZNEW(J)=ZNEW(J)+SUM(J)
    Y*Y+DELT
    KOUNT=KOUNT+1
    IF(KOUNT.EQ.IPRINT)CALL I0DATA(ZNEW,N*2)
    CALL DERFIN(ZNEW)
    IF(TFIN.GE.TLOGIC)RETURN
    IF(KOUNT.GE.ISTEP)RETURN
    GO TO 499
END
APPENDIX F

SOURCE PROGRAM FOR OBTAINING
OPTIMAL CONSTRAINTS AND FEEDFORWARD
CONTROL OF THE APPROXIMATE SYSTEM
***

**THIS PROGRAM USES THE GOLDEN SEARCH TECHNIQUE TO FIND THE CONSTRAINTS**

**ON THE CONTROL(S) AT A TIME OF THE APPROXIMATE SYSTEM, SUBROUTINE PBEW**

**IS USED TO CALCULATE THE INITIAL VALUES OF THE ADJOINT VARIABLE, THE**

**OPTIMAL PARAMETERS FOR THE TRANSFER FUNCTIONS ARE USED.**

* *

**COMMON IPRINT,KOUNT,DELT,Y,T1,FIN,TLOGIC,ISTEP**

1,J,H,TC(51),ZX(6),ZY(6),YLD,XCA(21),XCB(21),XT(21),GH,KJK
F1(CA,T)=A1*CA/EXP(9000.+T)
F3(CA,CB,T)=AP*CA/EXP(9000.+T)+BP*CB/EXP(15000.+T)+10.*TCST=T
1 /3.0

**DIMENSION P(6),RP(10)**

**DATA A1,B1,AP,BP,E1,E2,V,AH,BH,DZ,ALP/5.35E11,4.61E18,5.35E13,**

1 =2.305E20,9000.,15000.,0.10,100.,0.,0.05,0.33337

**TCST=316.4**

**READ THE INITIAL FEED CONDITIONS.**

**SOLVE THE STEADY STATE EQUATIONS TO OBTAIN THE BOUNDARY CONDITIONS ON**

**THE STATE VARIABLES.**

**CA=0.95**

**CB=0.05**

**T=331.4**

**DELZ=0.05**

**DO 2 N=1,20**

**AK1=DELZ*F1(CA,T)**
STORE THE BOUNDARY CONDITIONS

XCB(N) = CB
XT(N) = T
2 CONTINUE

READ THE INITIAL ESTIMATE OF THE ADJOINT VARIABLES

READ(5,5)(PP(I), I=1,4)
5 FORMAT(4F10.3)
WRITE(6,4)(PP(I), I=1,4)
4 FORMAT(1H1, 'INITIAL ASSUMPTION OF THE PARAMETERS' / 10X, 'PP(1) = ',
1 F10.3/10X, 'PP(2) = ', F10.3/10X, 'PP(3) = ', F10.3/10X, 'PP(4) = ')
2 , F10.3//}
DETERMINE THE LIMITS ON THE CONSTRAINTS AND START THE GOLDEN SEARCH TO FIND THE OPTIMAL CONSTRAINT ON THE CONTROL $\theta(t)$

XMIN=0.
XMAX=0.234
D=XMAX-XMIN
RESOL=D*1.0E-2
X1=XMIN+0.382*(XMAX-XMIN)
X2=XMIN+0.618*(XMAX-XMIN)
GH=X1

6 P(I)=PP(I)
KJK=0
WRITE(6,99)GH

SEARCH FOR THE INITIAL CONDITIONS ON THE ADJUNCT VARIABLES

CALL POW(PP,4,1,0,1.0*0.1,6,1)
CALL YIELD
WRITE(6,90)(TC(I),I=1,JM)
WRITE(6,56)YLD
Y1=YLD
SH=X2
DB 7 I=1,4

7 PP(I)=P(I)
KJK=0
WRITE(6,99)GH
CALL POW(PP,4,1,0,1.0*0.1,6,1)
CALL YIELD
WRITE(6,90)(TC(I),I=1,JM)
WRITE(6,5)(L
Y2=YL
DIFF=Y2-Y1
IF(DIFF*LT-5.0)GO TO 12
11 XMIN=X1
DX=ABS(X2-X1)
X1=X2
Y1=Y2
X2=XMAX-DX
GH=X2
DO 8 I=1,4
8 PPI(I)=P(I)
KJK=0
WRITE(6,99)GH
CALL P8M(PP,4,10,10,0,18,1)
CALL YIELD
WRITE(6,90)(TC(I)),I=1,JM)
WRITE(6,56)YLD
Y2=YLD
IF(X2-LT-X1)GO TO 13
14 IF(DX-LT-RESOL)GO TO 15
DIFF=Y2-Y1
IF(DIFF*LT-0.0)GO TO 12
GO TO 11
13 N=1
GO TO 16
12 XMAX=X2
DX=ABS(X2-X1)
X2=X1
Y2=Y1
X1=XMIN+DX
GH=X1
DO 9 I=1,4
9 PP(I)=P(I)
KJ=C
WRITE(6,39)
CALL PM(PP,4,1,U,1:1,6,1,2,1)
CALL YELL
WRITE(6,96)(TC(I),I=1,JM)
WRITE(6,56)YL
Y1=YL
IF(X2.LT.X1)G0 TO 17
18 IF(DX.LT.RESOL)G0 TO 15
DIFF=Y2-Y1
IF(DIFF.LT.0.0)G0 TO 12
G0 TO 11
17 N=N+2
16 XN=X2
X2=X1
X1=XN
XN=Y2
Y2=Y1
Y1=XN
G0 TO (14,18),N
15 IF(Y1.GT.Y2)G0 TO 19
G0 TO 10
19 Y2=Y1
X2=X1
10 Y2=Y2
WRITE(6,21)X1,X2,Y1,Y2
21 FORMAT(2(5X,F7.4),2(5X,F9.5))
WRITE(6,56)YL
WRITE(6,91)(ZY(I),I=1,4)
56 FORMAT(/9X,7HYIELD=,'F10.6/) 90 FORMAT(10(2X,F8.3))
91 FORMAT(4(2X,E12.5)/)
99 FORMAT(/10X,'GL=','F8.5/) 70 P
STOP
SUBROUTINE PRG(P,N, P)

THIS SUBROUTINE CALCULATES THE COST FOR SUBROUTINE PW.

COMMON IPRINT, COUNT, DELT, Y, T1, TFIN, TLOGIC, ISTEP
1 JM, TC(51), ZX(6), ZY(6), YLD, XCA(21), XCB(21), XT(21), GH, KJK
DIMENSION P(4,10)
DIMENSION ZNEW(8), Z(8), SUM(8), XK(8,8), FUN(8)
KJK=KJK+1

DEFINE THE INITIAL CONDITIONS ON THE ADJOINT VARIABLES

DO 1 I=1,4
1 ZX(I)=P(NR,I)
N=8
ICASE=2

START INTEGRATING THE SYSTEM OF THE STATE AND ADJOINT EQUATIONS UP TO THE FINAL TIME.

CALL RUNGA (Z, ZNEW, XK, SUM, FUN, N, ICASE)

OBTAIN THE FINAL VALUES OF THE ADJOINT VARIABLES AND COMPUTE THE COST FUNCTION WHICH MUST BE MINIMIZED.

DO 2 I=1,4
2 ZY(I)=ZNEW(I+4)
X1=ABS(ZNEW(5))
x2 = ABS(ZNEW(6))
x3 = ABS(ZNEW(7))
x4 = ABS(ZNEW(8))
P(NR, NP+1) = x1**2 + x2**2 + x3**2 + x4**2
RETURN
END
SUBROUTINE DEC1(U, E)

THIS SUBROUTINE DEFINES THE SYSTEM OF STATE AND ADJOINT DIFFERENTIAL
EQUATIONS TOGETHER WITH THE INITIAL CONDITIONS

COMMON IPRINT, KOUNT, DELT, Y, T1, TFIN, TLOGIC, ISTEP
1 * JM, TC(51), ZX(4), ZY(6), YLD, XCA(21), XCB(21), XT(21), GH, KJK
DIMENSION ZNEK(8), Z(8), SUM(8), XK(8, 8), FUN(8)
DIMENSION A(4, 5), B(4, 4), X(4)
DELT=5*D=2
Y=0.000
ISTEP=1000

INTRODUCE A STEP CHANGE IN THE FEED CONDITIONS

CA0=0.65/0.95=1.0

DEFINE THE OPTIMAL PARAMETERS FOR THE TRANSFER FUNCTION RELATING THE
OUTPUT TO THE FEED CONCENTRATION

TAU1=0.545
TAU2=0.547
TAU3=0.625
TAU4=0.626
GNA=1.0*0.83157
TAP=TAU1*TAU2
TAS=TAU1+TAU2
TAPA=TAU3*TAU4
TAPS=TAU3+TAU4
SPECIFY THE UPPER CONSTRAINT BY THE CONTROL G2(t)

SL=0.2324

USE THE INITIAL VALUES OF THE I0J91NT VARIABLES

DO 29  I=1,4

29  Z(I+4)=ZX(I)
       A(1,1)=1.0
       A(1,2)=0.0
       A(1,3)=1.0
       A(1,4)=0.0
       A(2,1)=0.0
       A(2,2)=1.0
       A(2,3)=0.0
       A(2,4)=1.0
       A(3,1)=1.0/TAPA
       A(3,2)=TAPS/TAPA
       A(3,3)=1.0/TAP
       A(3,4)=TAS/TAP
       A(4,1)=TAPS/(TAPA**2.0)
       A(4,2)=(TAPS/TAPA)**2.*1.0/TAPA
       A(4,3)=TAS/(TAPA**2.*)
       A(4,4)=(TAS/TAP)**2.*1.0/TAP
       A(1,5)=0.0
       A(2,5)=0.0
       IF(Z(8).LT.0.0)GO TO 19
       A(3,5)=CA9/TAPA+GH
       A(4,5)=CA9*TAPS/(TAPA**2.*)+GH*TAS/TAP
       GO TO 18

19  A(3,5)=CA9/TAPA+GL
       A(4,5)=CA9*TAFS/(TAPA**2.*)+3L*TAS/TAP
START SOLVING THE SYSTEM OF FOUR LINEAR EQUATIONS IN FOUR UNKNOWNS TO OBTAIN THE INITIAL CONDITIONS ON THE STATE AND ADJOINT VARIABLES OF THE APPROXIMATE SYSTEM.

18 NN=4
20 M=NN+1
105 IF(A(I,J))=111,106,111
106 KK=M=1
107 DO 109 I=2,KK
109 IF(A(I,J))=107,109,107
108 DO 108 J=1,M
107 TEMP=A(I,J)
108 A(I,J)=TEMP
110 CONTINUE
109 WRITE(6,110)
110 FORMAT(19H0N0 UNIQUE SOLUTION)
111 DO 112 J=2,M
112 DO 112 I=2,NN
113 B(I,J-1)=A(I,J)-A(I,J-1)*A(I,1)/A(1,1)
114 M=M-1
115 DO 114 J=1,M
116 DO 114 I=1,NN
117 A(I,J)=B(I,J)
118 IF(M=1)105,116,105
119 DO 117 I=1,NN
120 Z(I)=A(I,1)
117 X(I)=A(I,1)
118 RETURN

DEFINE THE STATE AND THE ADJOINT EQUATIONS

ENTRY DER(Z,FUN)

CHECK FOR THE TIME DELAY IN THE FEED CONCENTRATION

IF(Y*GT.1.06072)GO TO 1
G1=CA8/TAPA
JM=Y/DELT+1.1

CHECK THE SIGN OF THE FOURTH ADJOINT VARIABLE(P4)

1 IF(Z(8)*LT.0.0)GO TO 3
G2=GH
G0 TO 4
3 G2=GL
G0 TO 4
1 G1=(1.0*GNA)*CA8/TAPA
JM=Y/DELT+1.1
IF(Z(8)*LT.0.0)GO TO 6
G2=GH
G0 TO 4
6 G2=GL
4 FUN(1)=Z(2)
FUN(2)=TAPS*Z(2)/TAPA-Z(1)/TAPA+G1
FUN(3)=Z(4)
FUN(4)=Z(3)/TAPA-Z(4)*TAS/TAP+G2
FUN(5)=Z*(Z(1)+Z(3)+Z(6))/TAPA
FUNCTIONS:

\[
\begin{align*}
F(6) &= Z(5) + TAPS \times Z(2) / TAP, \\
F(7) &= Z(7) + Z(8) \times TAP / TAP, \\
F(8) &= Z(7) + Z(8) \times TAPS / TAP.
\end{align*}
\]

STORE THE OPTIMAL DIMENSIONLESS CONTROL, \(G_2(T)\):

\[
TC(J) = G_2 \\
\text{RETURN}
\]

CHECK FOR THE STOPPING CONDITION:

ENTRY DERFIN(Z)

TLGIC = 2.0
TFIN = 1.0
IF (Y \geq 2.47) TFIN = 3.0
RETURN
END
DEFINE THE NEW FEED CONDITIONS

3 CONTINUE
   TT(1) = TT(I)
   BCT(I) = BCT(I)
   ACT(I) = ACT(I)
   T(I) = T(I)
   CBT(I) = CBT(I)
   CART(I) = CART(I)
   DO 3, I = 2, 10, 20

USE THE STORED INITIAL CONDITIONS ON THE STATE VARIABLES

- E = 3.33E20, 900000, 150000, 3.10, 10000, 0.10, 1000, 0.5, 0.25
- DATA AL, BL, AB, BL, AE, BE, A/2, AP, A/2, BP, AP, A/2, AP, 5, 35E1, 4, 35E1, 4
- DIMENSION CAT(2), CBT(2), TT(2), CAN(2), CBN(2), T(I)
- COMMON IPRINT, X, Y, Z, DELT, Y, Z, TFIN, TLOGIC, ISTEP

PROGRAM

COMMUTATIVE FIELD WHICH IS MAXIMIZED BY THE GOLDEN SEARCH IN THE MAIN
THIS SUBROUTINE USES THE OPTIMAL NETURAL 2 CALCULATE THE
SOLUTION FIELD
T3 = 331.4
DT = 1.0 * DZ
AL = ALP * DT / 2
VIZ = V * DT / DZ
AMV = 1.0 * VTZ
APV = 1.0 * VTZ
TM = 0.*

DEFINE THE OPTIMAL PARAMETERS FOR THE TRANSFER FUNCTION RELATING THE EXIT CONCENTRATION OF B TO THE CONTROL

GN = 1.0 = 0.65970
TAU1 = 0.545
TAU2 = 0.547

OBTAIN THE OPTIMAL TEMPERATURE OF THE COOLING WATER FROM THE OPTIMAL DIMENSIONLESS CONTROL G2(I)

DO 44 I = 1, 50
TM = TM + DT
IF(TM * GT 9.35) G8 TO 6
U(I) = TC(I) * TAU2 * TAJ1
TC(I) = 95 * U(I) + 316.4
G8 TO 44
6  U(I) = TC(I) * TAU1 * TAJ2 + GN * U(I) * 18
TC(I) = 95 * U(I) + 316.4
44 CONTINUE
TM = 0.*

SOLVE THE STATE EQUATIONS FORWARD IN TIME AND STORE THE STATE VARIABLES
AT EACH GRID PRINT

DU 2 N=1,30
TM=TM+DT
60 DU 30 I=1,20
CAH(I)=CAT(I)
CBH(I)=CBT(I)
80 TN(I)=TT(I)
D8 13 K=1,6
CAH=(2*CAH+CAN(I)+CAT(I))/4*
CBH=(2*CBH+CBN(I)+CBT(I))/4*
TH=(2*T8+TN(I)+TT(I))/4*
PAL=9000*/TH
S8N=15000*/TH
IF(PAL*GT;60*)PAL=60*
IF(S8N*GT;60*)S8N=60*
XK1=A1/(10**EXP(PAL))
XK2=B1/(10**EXP(S8N))
CAT(I)=(2*VTZ*CAH+AMV*CAN(I)+2*TK1*CAH*DT)/APV
CBT(I)=(2*VTZ*CBH+AMV*CBN(I)+2*(TK1*CAH*XK2*CBH)*DT)/APV
13 TT(I)=(2*VTZ*T8+AMV*TN(I)+2*DT*(AH*XK1*CAH+BH*XK2*CBH+
1
ALP*(TC(N)+TH))/APV
D8 16 I=2,20
K=0
CAH=(CAN(I)+CAT(I))/2*
CBH=(CBN(I)+CBT(I))/2*
TH=(TN(I)+TT(I))/2*
81 PAL=9000*/TH
S8N=15000*/TH
IF(PAL*GT;60*)PAL=60*
IF(S8N*GT;60*)S8N=60*
XK1=A1/(10**EXP(PAL))
XK2=B1/(10**EXP(S8N))
\[
\begin{align*}
\text{CAT}(I) &= (\text{APV} \cdot \text{CAN}(I-1) + \text{AMV} \cdot \text{CAN}(I) + 2 \cdot X \cdot \text{CAH} \cdot \text{DT}) \cdot \text{AMV} \cdot \text{CAT}(I-1) \div \text{APV} \\
\text{CBT}(I) &= (\text{APV} \cdot \text{CBN}(I-1) + \text{AMV} \cdot \text{CBN}(I) + 2 \cdot (X \cdot \text{CAH} \cdot \text{XK} \cdot \text{C3H}) \cdot \text{DT}) \cdot \text{AMV} \cdot \text{CBT}(I-1) \\
\text{TT}(I) &= (\text{APV} \cdot \text{TNN}(I-1) + \text{AMV} \cdot \text{TNN}(I) + 2 \cdot \text{DT} \cdot (\text{AH} \cdot \text{XK1} \cdot \text{CAH} + 3 \cdot \text{XK2} \cdot \text{C3H} + \text{ALP} \cdot \text{TNN})(I-1)) \div \text{APV} \\
\text{CAH} &= (\text{CAN}(I-1) + \text{CAN}(I) + \text{CAT}(I-1) + \text{CAT}(I)) \div 4. \\
\text{CBH} &= (\text{CBN}(I-1) + \text{CBN}(I) + \text{CBT}(I-1) + \text{CBT}(I)) \div 4. \\
\text{TH} &= (\text{TNN}(I-1) + \text{TNN}(I) + \text{TT}(I-1) + \text{TT}(I)) \div 4. \\
\text{IF}(K=4) &= \text{31, 16, 15} \\
\text{DB} 70 &= I=1, 20 \\
\text{CBS}(I, N) &= \text{CBT}(I) \div 0.95 \\
\text{CONTINUE} \\
\text{END}
\end{align*}
\]

CALCULATE THE CUMMULATIVE YIELD OF B

\[
\text{CGL} = 0 \\
\text{DB} 55 &= I=2, 49 \\
\text{CBL} &= \text{CGL} \div \text{CBS}(20, I) \\
\text{YLD} &= \text{DT} \div (\text{CBS}(20, 1) + 2 \cdot \text{CBL} + \text{CRS}(20, 59)) \div 2 \\
\text{RETURN} \\
\text{END}
\]
APPENDIX G

SOURCE PROGRAM FOR OPTIMAL
THREE FEEDBACK SENSORS CONTROLLER
* THIS PROGRAM OBTAINS THE OPTIMAL PARAMETERS FOR A THREE FEEDBACK SENSORS CONTROLLER USING SUBROUTINE PB.*

```
COMMON xCA(21),xCB(21),XT(T1),TC(51),Z(51),CBO,LC1,LC2,LC3
1 ,FB1,FB2,FB3
F1(CA,T)=A1*CA/EXP(9000./T)
F2(CA,CB,T)=A1*CA/EXP(9000./T)*B1*CB/EXP(15000./T)
F3(CA,CB,T)=A1*CA/EXP(9000./T)*B1*CB/EXP(15000./T)+10*(TCST-T)
1 /3.0
DATA A1,B1,AP,BP,E1,E2,V,AH,BH,DZ,ALP/5.35E11,4.61E18,5.35E13
DATA 2,305E20,9000,15000,0,10,100,50,0.05,0.3333/
DATA NP,BB,AM,STEP,NPRNT/6,5,100,1,3,1/
DIMENSION PP(10)
TCST=316.4
DELZ=0.05

READ THE INITIAL FEED CONDITIONS.
SOLVE THE STEADY STATE EQUATIONS TO OBTAIN THE BOUNDARY CONDITIONS ON.
THE STATE VARIABLES.

CA=0.95
CB=0.05
T=331.4
ZL=0.
LS=0.
DB2 N=1,20
AK1=DELZ*F1(CA,T)
```
\[ \begin{align*}
AP1 &= \text{DEL}2*F1(CA, CH, T) \\
AP2 &= \text{DEL}2*F2(CA, CH, T) \\
AK1 &= \text{DEL}2*F3(CA, CH, T) \\
AP2 &= \text{DEL}2*F1(CA+AK1/2, T+AQ1/2) \\
AP3 &= \text{DEL}2*F2(CA+AK1/2, CB+AP1/2, T+AQ1/2) \\
AG2 &= \text{DEL}2*F3(CA+AK1/2, CB+AP1/2, T+AQ1/2) \\
AK3 &= \text{DEL}2*F1(CA+AK2/2, T+AP2/2) \\
AP3 &= \text{DEL}2*F2(CA+AK2/2, CB+AP2/2, T+AP2/2) \\
AG2 &= \text{DEL}2*F3(CA+AK2/2, CB+AP2/2, T+AP2/2) \\
AK4 &= \text{DEL}2*F1(CA+AK3, T+AQ3) \\
AP4 &= \text{DEL}2*F2(CA+AK3, CB+AP3, T+AQ3) \\
AG4 &= \text{DEL}2*F3(CA+AK3, CB+AP3, T+AQ3) \\
CA &= CA+(AK1+2*AK2+2*AK3+AK4)/6 \\
CB &= CB+(AP1+2*AP2+2*AP3+AP4)/6 \\
T &= T+(AQ1+2*AQ2+2*AQ3+AQ4)/6
\end{align*} \]

STORE THE BOUNDARY CONDITIONS

\[ \begin{align*}
XCA(N) &= CA \\
XCB(N) &= CB \\
XT(N) &= T
\end{align*} \]

2 CONTINUE
KJK = 0

ESTIMATE THE INITIAL VALUES OF THE CONTROLLER PARAMETERS

\[ \begin{align*}
PP(1) &= 60. \\
PP(2) &= 30. \\
PP(3) &= 325. \\
PP(4) &= 5.0
\end{align*} \]
REAL IN THE LOCATIONS OF THE FEEDBACK SENSORS

READ(5,91)LBC1, LBC2, LBC3
91 FORMAT(3(I2))
WRITE(6,92)LBC1, LBC2, LBC3
92 FORMAT(3(I5))

START THE SEARCH FOR THE PARAMETERS

CALL PBW(PP,4,3.0,30.,0.5,9,1)
WRITE(6,90)(TC(I),I=1,50)
90 FORMAT(10(2X,F8.4))
STOP
END
THIS SUBROUTINE USES THE CALCULATED PARAMETERS FROM SUBROUTINE RDN TO
COMPUTE THE COST FUNCTION WHICH MUST BE MINIMIZED.

DIMENSION P(4,16)
COMMON XCA(21),XCB(21),XT(21),TC(51),KJK,LBC
1 ,LBC1,LBC2,LBC3
DIMENSION CAT(21),CBT(21),TT(21),CAN(21),CBN(21),TN(21),CBS(21,51)
1 ,ACT(21),BCT(21),TCT(21)
DATA A1,AP,AP,BP,E1,E2,V,AH,BH,DZ,ALP,5.35E11,4.61E18,5.35E13,
1 -2.305E20,9.000,15.000,0.10,1.00,0.50,0.05,0.33333/
KJK=KJK+1

DEFINE THE CONTROLLER PARAMETERS

FB1=P(NR,1)
FB2=P(NR,2)
FB=P(NR,1)
BON=P(NR,2)

USE THE STORED INITIAL CONDITIONS

DB 3 I=1,20
CAT(I)=XCA(I)
CBT(I)=XCB(I)
TT(I)=XT(I)
ACT(I)=CAT(I)
BCT(I)=CBT(I)
TCT(I)=TT(I)
3 CONTINUE

SPECIFY THE NEW FEED CONDITIONS

CA9=0.65
CB9=0.05
TF=331.4
DT=10*DZ
ALT=ALP*DT/2
VTZ=V*DT/DZ
AMV=1.0*VTZ
APV=1.0+VTZ
TM=0.0
KTP=0
LAST=0
IF(JM*NE.0)LAST=1
DB 9 N*1.50
TM=TM+DT

DEFINE THE FEEDBACK CONTROL AS A FUNCTION OF CONCENTRATIONS

IF(N.EQ.1)GO TO T9 4
TC(N)=CN*FB1*CBS(L0C1,N-1)+FB2*CBS(L0C2,N-1)+FB3*CBS(L0C3,N-1)
GO TO 60
4 TC(N)=CN*FB1*CBT(L0C1)+FB2*CBT(L0C2)+FB3*CBT(L0C3)

START SOLVING THE STATE EQUATIONS

60 DB 50 I=1,20
214

CAN(I)=CAT(I)
CBN(I)=CBT(I)

XU TN(I)=TT(I)
DB 13 K=1,6
CAH=(2*C89+CAN(I)+CAT(I))/4*
CBH=(2*C89+CBN(I)+CBT(I))/4*
TH=(2*TB+TN(I)+TT(I))/4*
PAL=9000*/T-
SBN=15000*/TH
IF(PAL>ST=60)PAL=60*
IF(SBN>ST=60)SBN=60*
XK1=A1/(10**EXP(PAL))
XK2=B1/(10**EXP(SBN))
CAT(I)=(2*VTZ*CAR+AV*CAN(I)+2*XK1*CAH*DT)/APV
CBT(I)=(2*VTZ*CB8+AV*CBN(I)+2*(XK1*CAH=XK2*CBH)*DT)/APV

13 TT(I)=(2*VTZ*TS+AV+TN(I)+2*DT*(AH*XK1*CAH+BH*XK2*CBH)+
ALP*(1C-TH))/APV

DB 16 I=2,20
K=0
CAH=(CAN(I)+CAT(I-1))/2*
CBH=(CBN(I)+CBT(I-1))/2*
TH=(TN(I)+TT(I-1))/2*

81 PAL=9000*/T-
SBN=15000*/TH
IF(PAL>ST=60)PAL=60*
IF(SBN>ST=60)SBN=60*
XK1=A1/(10**EXP(PAL))
XK2=B1/(10**EXP(SBN))
CAT(I)=(AV*CAN(I-1)+AMV*CAN(I)=2*XK1*CAH*DT=AMV*CAT(I-1))/APV
CBT(I)=(AV*CBN(I-1)+AMV*CBN(I)+2*(XK1*CAH=XK2*CBH)*DT=AMV*CBT(I-1))/APV

TT(I)=(AV*TN(I-1)+AV*TN(I)+2*DT*(AH*XK1*CAH+BH*XK2*CBH+ALP*
ALP*(1C-TH))/APV

CAH=(CAN(I)+CAN(I)+CAT(I-1)+CAT(I))/4*
CUB = (CUB(I+1) + CUB(I) + CUB(I-1) + CUB(I))/4.
TH = (TH(I-1) + TH(I) + TH(I+1) + TH(I))/4.
K = K + 1
IF(K = 4) THEN 13, 16
16 CONTINUE
DO 70 I = 1, 2
CBS(I, N) = CUB(I)
70 CONTINUE
9 CONTINUE

CALCULATE THE CUMULATIVE YIELD OF H

CBL = 0.
DO 55 I = 2, 49
55 CBL = CBL + CBS(20, I)
YLD = DT * (CBS(20, I) + 2 * CBL + CBS(20, 50))/2.

DEFINE THE COST FUNCTION

P(NR, NP + 1) = YLD
RETURN
END
VITA

Ahmad Shariat was born on March 21, 1945. After passing the entrance examination he entered the University of Tehran, Tehran, Iran in September 1963. He studied physics and mathematics for one year and came to the United States in September 1964.

After completing one term of English language and orientation, he entered Louisiana State University. He transferred to Tennessee Technological University, Cookeville, Tennessee in June 1965 where he received a B.S. in Chemical Engineering in 1967.

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EXAMINATION AND THESIS REPORT

Candidate: Ahmad Shariat

Major Field: Chemical Engineering

Title of Thesis: Optimal Control of a Distributed Parameter System

Approved:

[Signatures]

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination:

September 27, 1971