$$(\beta f_n - f_y) + \left\{ Le\left(\frac{\beta f_y}{Le} + f_n \right)^2 + (f_y - \beta f_n)^2 \right\}^{1/2} \leq \frac{\pi^2}{4}$$

or

$$\beta f_n - f_y + \left\{ Le\left(\frac{\beta f_y}{Le} - f_n \right)^2 + (\beta f_n + f_y)^2 \right\}^{1/2} \leq \frac{\pi^2}{4} \qquad \text{(D5)}$$

Define

$$S_1 = \beta f_n - f_y + \left\{ Le\left(\frac{\beta f_y}{Le} - f_n \right)^2 + (\beta f_n + f_y)^2 \right\}^{1/2}$$

Then

$$S_1 \geq \beta f_n - f_y + \{(\beta f_n + f_y)^2\}^{1/2} = 2\beta f_n \qquad \text{(D6)}$$

Condition (26) can be written as

$$\sup_{0 \leq x \leq 1} (2\beta f_n) < \frac{\pi^2}{4} \qquad \text{(D7)}$$

and Condition (D5) is equivalent to

$$\sup_{0 \leq x \leq 1} S_1 \leq \frac{\pi^2}{4} \qquad \text{(D8)}$$

From Conditions (D6), (D7), and (D8) it can be concluded that the Condition (D7) is less conservative than Condition (D8), that is, our result, Condition (26), is less conservative than the result obtained by Murphy and Crandall (1970).

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Approximation in Control of Nonlinear Dynamic Systems

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The type of system approximation in which the system state space x is mapped into a scalar domain V by a quadratic transformation

$$V = \frac{1}{2}\mathbf{x}'\mathbf{Q}\mathbf{x}$$

where Q is appropriately determined, is used to develop a suboptimal control procedure for unconstrained lumped parameter dynamic systems via the application of Pontryagin's Maximum Principle. The optimization problem in the scalar domain becomes an initial value problem when the scalar adjoint variable is held constant throughout the course of control. The resulting computational scheme includes an effective and simple way to construct the transformation matrix Q and a straightforward minimum seeking approach to locate the best constant overall average scalar adjoint parameter. For the class of problems with quadratic performance index, system equation approximation further reduces the determination of Q to the solution of a matrix Riccati equation.

The application of the proposed suboptimal control procedure to four chemical engineering systems shows that the procedure is simple, direct, and efficient and works particularly well for problems where the final time is large.

SCOPE

In establishing optimal control for nonlinear complex chemical engineering systems one usually turns to the Pontryagin's Maximum Principle. Recently, considerable effort has been directed towards developing means of solving the two point boundary value problem (TPBVP) resulting from the use of the maximum principle. In addition to the difficulty of solving the TPBVP, there are the difficulties of determining the initial control policy and of instability of the adjoint equations.

Suboptimal procedures have been therefore introduced recently to simplify the computational procedure. These are useful only if the resulting control policy is reasonably close to the optimal. The approximations frequently used in the suboptimal procedures include system equation approximation (such as linearization) and/or adjoint equation approximation.

Very promising results have been obtained by transforming the n-dimensional state space to a scalar domain by a quadratic transformation $V = \frac{1}{2}x'\,Q\,x$, thereby describing the state in terms of the scalar V. This simplifies the problem considerably, since now the adjoint equation becomes a scalar differential equation.

In this paper we employ system linearization and state transformation. Furthermore, we use an average adjoint

variable which can be held constant throughout the time interval. This converts the two point boundary value problem into an initial value problem, since no integration of the adjoint equation is necessary. The objective therefore is to develop a simple means of establishing optimal control for nonlinear systems.

CONCLUSIONS AND SIGNIFICANCE

This paper demonstrates a new algorithm for the solution of unconstrained control problems. The algorithm has been applied successfully to typical chemical engineering problems with both quadratic and nonquadratic performance indices. The procedure was found to be computationally stable and also efficient.

The essential feature of the method lies in keeping the adjoint constant throughout the course of control. This constant adjoint parameter eliminates the necessity to integrate the adjoint equation and simplifies the determination of the transformation matrix Q. Thus the overall computational effort is considerably reduced, and the best result is obtained simply by optimizing with respect to the constant adjoint parameter.

In fact, the procedure presents a practical way of optimizing dynamic systems. The low degree of suboptimality supports the potential usefulness of this approach. Further, it is shown that the adjoint can be held constant in the optimization of dynamic nonlinear systems with exceptionally good results for systems with large final times.

PROBLEM FORMULATION AND SUBOPTIMAL PROCEDURE

Consider the class of continuous-time nonlinear systems described by the vector differential equation

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x},\mathbf{u}), \quad \mathbf{x}(0) \text{ specified} \tag{1}$$

where $\mathbf{x}$ is an n-dimensional state vector and $\mathbf{u}$ is an r-dimensional control vector. The optimization problem *is to determine* the control policy $\mathbf{u}(t)$ over a specified time interval of

$$0 \leq t < t_f \tag{2}$$

so that the performance index

$$I = \int_0^{t_f} \varphi\,(\mathbf{x}, \mathbf{u})\, dt \tag{3}$$

is minimized.

The suboptimal procedure is approached by the construction of a quadratic functional, according to Schlossmacher and Lapidus (1971)

$$V = \frac{1}{2}\mathbf{x}'\mathbf{Q}\mathbf{x} \tag{4}$$

which maps the vector state space $\mathbf{x}$ into a scalar domain V by a $n \times n$ dimensional symmetric transformation matrix $\mathbf{Q}$. The optimization problem is thus simplified to the problem of the minimization of the performance index given in Equation (3) with respect to the transformed scalar system equation

$$\dot{V} = \dot{\mathbf{x}}'\mathbf{Q}\mathbf{x} \tag{5}$$

To obtain the solution to this problem a Hamiltonian is introduced and is defined as

$$H = z\dot{V} + \varphi \tag{6}$$

where z is a scalar adjoint variable. Substituting Equation (5) into Equation (6) yields

$$H = z\dot{\mathbf{x}}'\mathbf{Q}\mathbf{x} + \varphi \tag{7}$$

Assuming here that the Hamiltonian is twice differentiable with respect to the control and that the control is unconstrained, we may use the stationary condition

$$\frac{\partial H}{\partial \mathbf{u}} = \mathbf{0} \tag{8}$$

to give the minimizing suboptimal control

$$\mathbf{u}^* = \mathbf{u}(\mathbf{x}, z, \mathbf{Q}) \tag{9}$$

The adjoint equation is given by

$$\dot{z}(t) = -\frac{\partial H}{\partial V} \tag{10}$$

with boundary condition

$$z(t_f) = 0 \tag{11}$$

In this work, however, instead of integrating the adjoint equation, we approximate z to be a constant for the entire time interval. With a value for the constant adjoint parameter which is now denoted by $\hat{z}$, the problem is an initial value problem given in terms of Equations (1) and (8). Then a simple systematic procedure can be used to improve subsequent choice of $\hat{z}$ until the performance index given by Equation (3) is minimized. In effect we will thus use the best average value for the scalar adjoint. With this constant adjoint $\hat{z}$ the Hamiltonian becomes

$$H = \hat{z}\dot{\mathbf{x}}'\mathbf{Q}\mathbf{x} + \varphi \tag{7a}$$

and the suboptimal control becomes

$$\mathbf{u}^* = \mathbf{u}(\mathbf{x}, \hat{z}, \mathbf{Q}) \tag{9a}$$

Let us now consider the determination of the transformation matrix $\mathbf{Q}$. Since the overall system adjoint parameter is held constant, it follows that

$$\frac{\partial H}{\partial V} = 0 \tag{12}$$

This leads to the condition

$$\frac{\partial H}{\partial \mathbf{x}} = \mathbf{0} \tag{13}$$

which forms the basis for the determination of $\mathbf{Q}$. Partial differentiation of Equation (7a) with respect to $\mathbf{x}$ and imposing the stationary condition of suboptimal control yields

$$\hat{z}\left\{\frac{\partial \mathbf{f}'}{\partial \mathbf{x}} + \left(\frac{\partial \mathbf{u}'}{\partial \mathbf{x}}\right)\left(\frac{\partial \mathbf{f}'}{\partial \mathbf{u}}\right)\right\}\mathbf{Q}\mathbf{x} + \hat{z}\mathbf{Q}\,\mathbf{f}$$

$$+\frac{\partial\varphi}{\partial \mathbf{x}}+\left(\frac{\partial \mathbf{u}'}{\partial \mathbf{x}}\right)\left(\frac{\partial\varphi}{\partial \mathbf{u}}\right)=\mathbf{0} \quad (14)$$

Solution to this equation for the $\frac{1}{2}n\ (n+1)$ independent elements of $\mathbf{Q}$ can be easily performed by numerically minimizing the expression $(\partial H/\partial \mathbf{x})'\ (\partial H/\partial \mathbf{x})$. Although this way of determining $\mathbf{Q}$ for nonlinear systems is simpler than that of Cormack and Luus (1972), still the solution of Equation (14) could require considerable effort. We therefore consider an important class of problems where the performance index is quadratic, that is,

$$I=\int_0^{t_f}\frac{1}{2}\,(\mathbf{x}'\mathbf{S}\mathbf{x}+\mathbf{u}'\mathbf{R}\mathbf{u})\,dt \quad (15)$$

in which $\mathbf{S}$ is a symmetric positive semidefinite matrix and $\mathbf{R}$ is a symmetric positive definite matrix. The determination of $\mathbf{Q}$ by Equation (14) can then be further simplified by the incorporation of system equation approximation.

Pearson (1962) proposed the apparent linearization approximation to system equation in which Equation (1) is written in the form

$$\dot{\mathbf{x}}(t)=\mathbf{A}(\mathbf{x},\mathbf{u},t)\mathbf{x}+\mathbf{B}(\mathbf{x},\mathbf{u},t)\mathbf{u} \quad (16)$$

where $\mathbf{A}$ and $\mathbf{B}$ are respectively $n\times n$ and $n\times r$ dimensional matrices which are constructed from original system equations. Weber and Lapidus (1971) applied this approximation to solving chemical engineering systems and presented a way to select the coefficient matrices $\mathbf{A}$ and $\mathbf{B}$.

These matrices $\mathbf{A}$ and $\mathbf{B}$ are used to generate suboptimal controls. They are reevaluated at each instant when the state is established since they are functions of the states and the previous controls used to obtain the states. To show how $\mathbf{A}$ and $\mathbf{B}$ are calculated, suppose the numerical integration of the state Equation (1) has been carried for N steps; that is, the time $t=Nh$ has been reached, where h is the integration time step size, and $\mathbf{x}(N)=\mathbf{x}\ (t)$ has just been obtained. $\mathbf{A}$ and $\mathbf{B}$ are formed by supplying state $\mathbf{x}(N)$ and the control $\mathbf{u}(N-1)$ to give

$$\mathbf{A}=\mathbf{A}\,(\mathbf{x}(N),\mathbf{u}(N-1),N) \quad (17)$$

$$\mathbf{B}=\mathbf{B}\,(\mathbf{x}(N),\mathbf{u}(N-1),N) \quad (18)$$

The corresponding suboptimal control at $t=Nh$ is

$$\mathbf{u}^*(t)=\mathbf{u}(\mathbf{x}(N),\hat{z},\mathbf{Q}) \quad (19)$$

Following this way of evaluating $\mathbf{A}$ and $\mathbf{B}$, the suboptimal control derived from apparent linearization, which is now obtained by putting Equation (16) into Equation (7a) and using the stationary condition, Equation (8) is given by

$$\mathbf{u}^*=-\hat{z}\mathbf{R}^{-1}\mathbf{B}'\mathbf{Q}\mathbf{x} \quad (20)$$

Substituting Equations (16) and (20) into Equation (14) yields a general equation for the determination of $\mathbf{Q}$, namely,

$$\hat{z}\mathbf{A}'\mathbf{Q}+\hat{z}\mathbf{Q}\mathbf{A}-\hat{z}\mathbf{Q}\mathbf{B}\mathbf{R}^{-1}\mathbf{B}'\mathbf{Q}\hat{z}+\mathbf{S}=\mathbf{0} \quad (21)$$

Equation (21) is the matrix Riccati equation which can be readily solved.

Although apparent linearization can also be applied to problems associated with nonquadratic performance index, the effort of determining $\mathbf{Q}$ is not reduced since the resulting equation derived from Equation (14) is no longer the matrix Riccati equation. In this case, $\mathbf{Q}$ has to be evaluated by function-minimization; thus no advantage is obtained from the system equation approximation.

Since $\hat{z}$ and $\mathbf{Q}$ appear as the product $\hat{z}\mathbf{Q}$ in Equations (14) and (21), in the determination of $\mathbf{Q}$, $\hat{z}$ may be arbitrarily set at unity while $\mathbf{Q}$ is determined. In the determination of $\mathbf{Q}$, the state $\mathbf{x}$ and the control $\mathbf{u}$ are required. In Equation (14), the control $\mathbf{u}$ is expressed as a function of $\mathbf{x}$, $\hat{z}$, and $\mathbf{Q}$ by Equation (9a). Although it is desirable to use a state $\mathbf{x}$ which is characteristic of the dynamic system, it is also reasonable to choose a state which is within in the region of dynamic response of the system. For the cases when the problem is associated with quadratic performance index and the objective is to minimize state deviations and control effort, the state $\mathbf{x}=\mathbf{0}$ is found to be satisfactory in Equation (21), while at other times it is better to use $\mathbf{x}=\mathbf{x}(0)$ in order to avoid numerical instability. Then, the corresponding control at $t=0$, $\mathbf{u}(0)$ may be approximated by solving $\mathbf{f}(\mathbf{x}(0),\mathbf{u}(0))=\mathbf{0}$; that is, $\mathbf{u}(0)$ is the control which holds the state at $\mathbf{x}(0)$.

Having determined $\mathbf{Q}$, we may then improve the overall result by searching for the best $\hat{z}$ which will give the lowest performance index. Even though various one dimensional search procedures may be used to obtain the best value of $\hat{z}$, the combination of one dimensional hillclimbing and quadratic approximation is found to be most efficient. The initial choice of $\hat{z}$ is easily obtained from Equation (14) or (21) at the initial state with $\mathbf{u}(0)$ evaluated in the above-mentioned manner. At this starting value of $\hat{z}$, the associated performance index is obtained by integrating Equations (1) and (3) with control given by Equation (9a). Another adjoint parameter is then selected by stepping from the starting adjoint in the direction such that at a new value of $\hat{z}$ the corresponding performance index I decreases relative to the starting one. We continue incrementing or decrementing the value of the adjoint in this manner, adjusting the step size in accordance to the relative difference of the last two values of I until the performance index no longer decreases. At this point we may approximate the dependence of I on $\hat{z}$ by a quadratic function

$$I=c_1+c_2\hat{z}+c_3\hat{z}^2 \quad (22)$$

and use the last three values of $\hat{z}$ and the corresponding values of I to determine the constants c_1, c_2, and c_3. The best $\hat{z}$ which gives the minimum I is

$$\hat{z}^*=-\frac{c_2}{2c_3} \quad (23)$$

To evaluate such a procedure which eliminates the need to integrate adjoint equations, we present the computational results of four typical chemical engineering systems.

TEST SYSTEMS

Nonlinear Gas Absorber

The six-plate gas absorption tower was first studied by Lapidus and Amundson (1950). Weber and Lapidus (1971) used this system to demonstrate the use of apparent linearization. In normalized form, the state equations are

$$\dot{x}_1 = \{-(40.8 + 66.7(m_1 + 0.08\,x_1))\,x_1 + 66.7(m_2 + 0.08\,x_2)\,x_2 + 40.8\,u_1\}/w_1$$

$$\dot{x}_i = \{40.8\,x_{i-1} - (40.8 + 66.7(m_i + 0.08\,x_i))\,x_i + 66.7(m_{i+1} + 0.08\,x_{i+1})\,x_{i+1}\}/w_i, \quad i = 2, 3, 4, 5 \quad (24)$$

$$\dot{x}_6 = \{40.8\,x_5 - (40.8 + 66.7(m_6 + 0.08\,x_6))\,x_6 + 66.7\,(m_7 + 0.08\,u_2)\,u_2\}/w_6$$

with

$$w_i = (m_i + 0.16\,x_i) + 75, \quad i = 1, 2, \ldots, 6 \quad (25)$$

and the vector $\mathbf{m}$ is

$$\mathbf{m} = \begin{bmatrix} 0.7358 \\ 0.7488 \\ 0.7593 \\ 0.7677 \\ 0.7744 \\ 0.7797 \\ 0.7838 \end{bmatrix} \quad (26)$$

The initial state is

$$\mathbf{x}(0) = \begin{bmatrix} -0.0342 \\ -0.0619 \\ -0.0837 \\ -0.1004 \\ -0.1131 \\ -0.1224 \end{bmatrix}$$

and the performance index to be minimized is

$$I = \int_0^{t_f} (\mathbf{x}'\mathbf{x} + \mathbf{u}'\mathbf{u})\,dt \quad (27)$$

With apparent linearization applied to this system and using the coefficient matrices $\mathbf{A}$ and $\mathbf{B}$ as constructed by Weber and Lapidus, the suboptimal controls are

$$u_1^* = -\frac{1}{2}\,\hat{z}\,(\mathbf{Qx})_1\,b_{11} \quad (28)$$

$$u_2^* = -\frac{1}{2}\,\hat{z}\,(\mathbf{Qx})_2\,b_{26} \quad (29)$$

CSTR with Proportional Control

Details of this dynamic system are given by Lapidus and Luus (1967). In normalized and dimensionless form, the system equations are

$$\dot{x}_1 = -\exp\left(\frac{25x_2}{x_2 + 2}\right)(x_1 + 0.5) - x_1 + 0.5$$

$$\dot{x}_2 = \exp\left(\frac{25x_2}{x_2 + 2}\right)(x_1 + 0.5) - kx_2\,(x_2 + 0.25) - 2x_2 - 0.5 + u \quad (30)$$

Here x_1 and x_2 are the normalized dimensionless concentration and temperature, and k is the proportional control constant. The control variable u is the controlled coolant flow. The performance index to be minimized is

$$I = \int_0^{t_f} (\mathbf{x}'\mathbf{x} + u^2)\,dt \quad (31)$$

and $t_f = 5$.

Various values of the proportional control constant are investigated in this work. When

$$k = 0.0, \quad \mathbf{x}(0) = \begin{bmatrix} 0.09 \\ -0.04 \end{bmatrix}$$

$$k = 8.9, \quad \mathbf{x}(0) = \begin{bmatrix} -0.1111889 \\ 0.0322358 \end{bmatrix}, \quad \begin{bmatrix} -0.15 \\ 0.05 \end{bmatrix}$$

$$k = 20.0, \quad \mathbf{x}(0) = \begin{bmatrix} -0.1111889 \\ 0.0322358 \end{bmatrix}$$

When $k = 8.9$, two initial states are given, the first one is on limit cycle and the second one is outside the limit cycle. The suboptimal control is

$$u^* = -\frac{1}{2}\,\hat{z}\,(q_{12}\,x_1 + q_{22}\,x_2) \quad (32)$$

This system is also used to show the incorporation of apparent linearization to the proposed suboptimal control procedure. The coefficient matrices $\mathbf{A}$ and $\mathbf{B}$ are also given by Weber and Lapidus (1971).

Nonlinear Exothermic CSTR

This system is the same as that of the proportional control CSTR except that the second state equation is written as

$$\dot{x}_2 = -(u + 2)\,(x_2 + 0.25) + (x_1 + 0.5)\exp\left(\frac{25x_2}{x_2 + 2}\right) \quad (33)$$

and the performance index is

$$I = \int_0^{t_f} (\mathbf{x}'\mathbf{x} + 0.1\,u^2)\,dt \quad (34)$$

with $t_f = 0.78$. The suboptimal control is

$$u^* = 5\,\hat{z}\,(x_2 + 0.25)\,(q_{12}\,x_1 + q_{22}\,x_2) \quad (35)$$

Pressure Control Plug-Flow Tubular Reactor

The system which represents the reaction $A \rightarrow 2B \rightarrow C$ occurring in the tubular reactor was first studied by Lee (1968). The state equations are

$$\dot{x}_1 = -\frac{2k_1u}{(d + x_2)}$$

$$\dot{x}_2 = \frac{4k_1ux_1}{(d + x_2)} - \frac{4k_2u^2x_2^2}{(d + x_2)^2} \quad (36)$$

where x_1 and x_2 represent the concentrations of A and B in the reactor. The constants are

$$k_1 = 0.01035 \text{ g-mole/(liter-min-atm)}$$

$$k_2 = 0.04530 \text{ g-mole/(liter-min-atm}^2\text{)}$$

$$d = 2\,x_1(0) + x_2(0)$$

The initial state vector is

$$\mathbf{x}(0) = \begin{bmatrix} 0.0105 \\ 0.0085 \end{bmatrix}$$

Pressure is the control variable. The goal is to maximize the output concentration of B, that is, the performance index to be minimized is

$$I = -x_2\,(t_f) \quad (37)$$

The time interval of control is 8 minutes. The suboptimal control is

$$u^* = \frac{k_1x_1\,(d + x_1)\,\{-\hat{z}\,(\mathbf{Qx})_1 + 2\hat{z}\,(\mathbf{Qx})_2 - 2\}}{4\,k_2x_2^2\,(\hat{z}(\mathbf{Qx})_2 - 1)} \quad (38)$$

Table 1. Performance Indices for Nonlinear Gas Absorber

$h = 0.2$

Method	t_f	I	Percentage subop-timality	z^*	No. of iter-ations	Compu-tation time
Optimal	5	0.1124			6	1.8
This work	5	0.1137	1.15	0.7047	7	1.2
FFT	5	0.1124	0.00			2.0
Optimal	10	0.1279			7	3.6
This work	10	0.1283	0.31	0.9470	6	1.5
FFT	10	0.1284	0.39			6.8
Optimal	14	0.1296			8	6.6
This work	14	0.1296	0.00	0.9886	6	1.9
FFT	14	0.1296	0.00			12.5
Optimal	20	0.1299			9	10.4
This work	20	0.1299	0.00	1.0010	6	2.3
FFT	20	0.1299	0.00			24.8

NUMERICAL RESULTS AND DISCUSSION

For all systems the optimal performance index is obtained by the second variational method (Luus and Lapidus, 1967) and is used for comparison with the suboptimal performance index. Computations were done on the IBM 370/165 computer and computing times are reported in seconds. The standard Runge-Kutta-Gill integration procedure is used for numerical integration. Unless otherwise stated, $\mathbf{u}(0)$, which is used in the determination of $\mathbf{Q}$, is obtained by solving $\mathbf{f}(\mathbf{x}(0), \mathbf{u}(0)) = \mathbf{0}$. The Rosenbrock hillclimbing numerical minimization procedure is used for solving Equation (14). The proximity of the suboptimal performance index I to the optimal index I° is given by the degree of suboptimality which is defined as

$$\text{Percentage suboptimality} = \frac{I - I^\circ}{I^\circ} \times 100\% \qquad (39)$$

The nonlinear gas absorber is first studied with final times of $t_f = 5$, 10, 14, and 20 minutes. The transformation matrix $\mathbf{Q}$ is obtained by Equation (21) with matrices $\mathbf{A}$ and $\mathbf{B}$ evaluated at $\mathbf{x}(0)$ and $\mathbf{u}(0)$. The matrix is

$$\mathbf{Q} = \begin{bmatrix} 1.1284 & 0.7958 & 0.5647 & 0.3831 & 0.2308 & 0.1017 \\ 0.7958 & 1.8306 & 1.3287 & 0.9129 & 0.5540 & 0.2452 \\ 0.5647 & 1.3287 & 2.2240 & 1.5480 & 0.9479 & 0.4221 \\ 0.3831 & 0.9129 & 1.5480 & 2.2647 & 1.4007 & 0.6286 \\ 0.2308 & 0.5540 & 0.9479 & 1.4007 & 1.9153 & 0.8703 \\ 0.1017 & 0.2452 & 0.4221 & 0.6286 & 0.8703 & 1.1176 \end{bmatrix} \qquad (40)$$

Results from this work are compared with the optimal performance indices and those obtained from the Finite Final Time (FFT) method of Weber and Lapidus. Table 1 summarizes the results obtained with the integration time step-size $h = 0.2$.

At the final time of $t_f = 5$, the performance index obtained by the proposed method differs considerably from the optimal one (percentage suboptimality = 1.15). This is due to the higher control effort obtained by this suboptimal procedure which drives the state to $\mathbf{x} = \mathbf{0}$. Figure 1 compares the difference in the state dynamics of the plate 6 composition obtained by this work and that by the second variational method. For large final time, for example, $t_f = 20$, Weber and Lapidus (1971) reported on the difficulty of using quasilinearization procedure to optimize the nonlinear gas absorber. The reason is given by the stiff differential equations associated in the quasilinearization algorithm. In the proposed suboptimal control procedure, no computational difficulty is encountered and the method is shown to work very well for large t_f.

When $t_f = 14$, the work of Schlossmacher (1969) is included for the comparison of the suboptimal control policies which is shown in Figure 2. The control sequence obtained by Schlossmacher is discrete; however, for the plotting of control variable versus time, smooth curve is

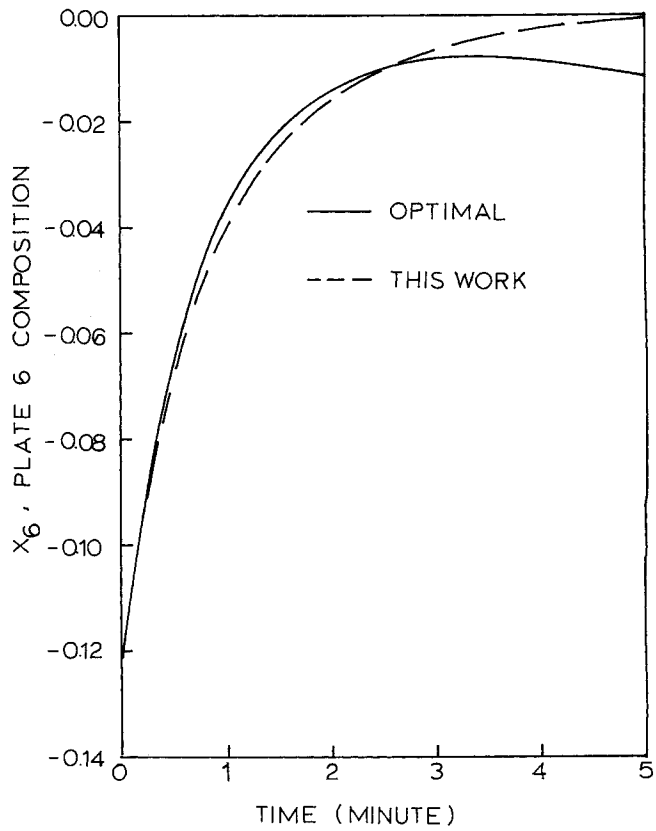

Fig. 1. Dynamics of x_6 of nonlinear gas absorber, $t_f = 5$.

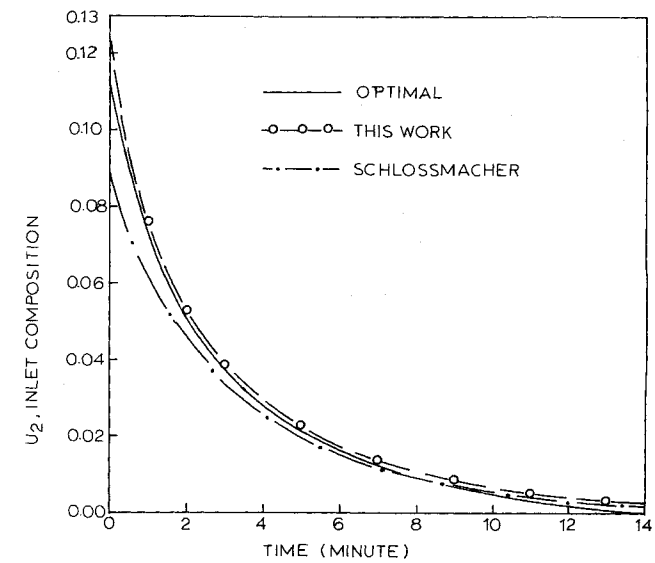

Fig. 2. Control policy for nonlinear gas absorber, $t_f = 14$.

drawn through the controls at their values at the beginning of every time step. Control sequence from Weber and Lapidus is not shown because it is very close to the optimal control policy. The apparently lower control effort obtained by Schlossmacher leads to a higher performance index of 0.1580.

The second example is the CSTR with proportional control. In all cases of different k's, the transformation matrices are evaluated at $\mathbf{x} = \mathbf{0}$ and $\mathbf{u} = \mathbf{0}$. When $k = 20$ the matrix is given by

$$\mathbf{Q} = \begin{bmatrix} 0.4019 & -0.1889 \\ -0.1889 & 1.8156 \end{bmatrix} \tag{41}$$

and when $k = 8.9$,

$$\mathbf{Q} = \begin{bmatrix} 0.7475 & 0.5758 \\ 0.5758 & 6.5268 \end{bmatrix} \tag{42}$$

with $k = 0.0$ the transformation matrix is

$$\mathbf{Q} = \begin{bmatrix} 0.9889 & 1.6727 \\ 1.6727 & 14.4470 \end{bmatrix} \tag{43}$$

Results which include those obtained by the FFT method are presented in Table 2. Computational efforts in both suboptimal procedures are approximately the same with $h = 0.1$, but the results of this work are closer to optimum. At smaller value of h, the proposed method is computationally more efficient, as is shown in the second part of the table with $h = 0.025$. Figure 3 shows a typical phase plane trajectory when $k = 0.0$.

Numerical instability resulting at large t_f is not only observed for the quasilinearization procedure but the same difficulty is encountered with the use of the second variational method. As shown in Figure 3, the states al-

TABLE 2. PERFORMANCE INDICES FOR PROPORTIONAL CONTROL CSTR

Method	k	I	Percentage subop-timality	z^*	No. of iter-ations	Compu-tation time
		$h = 0.1$				
This work	0.0	0.009641		0.9959	12	0.5
FFT	0.0	0.009704				0.4
This work	8.9*	0.005393		0.7476	5	0.3
FFT	8.9*	0.005423				0.4
This work	8.9**	0.010456		0.8098	12	0.5
FFT	8.9**	0.010598				0.4
This work	20.0	0.003832		0.7462	5	0.3
FFT	20.0	0.003833				0.4
Optimal	20.0	0.003833				
		$h = 0.025$				
This work	0.0	0.009637	0.07	0.9959	12	1.9
FFT	0.0	0.009630	0.00			4.3
Optimal	0.0	0.009630				
This work	8.9*	0.005391	0.02	0.7476	5	0.8
FFT	8.9*	0.005405	0.28			4.3
Optimal	8.9*	0.005390				
This work	8.9**	0.010454	0.05	0.8098	12	1.9
FFT	8.9**	0.010551	0.97			4.3
Optimal	8.9**	0.010449				
This work	20.0	0.003830	0.05	0.7462	5	0.8
FFT	20.0	0.003830	0.05			4.3
Optimal	20.0	0.003828				

* On limit cycle.
** Outside limit cycle.

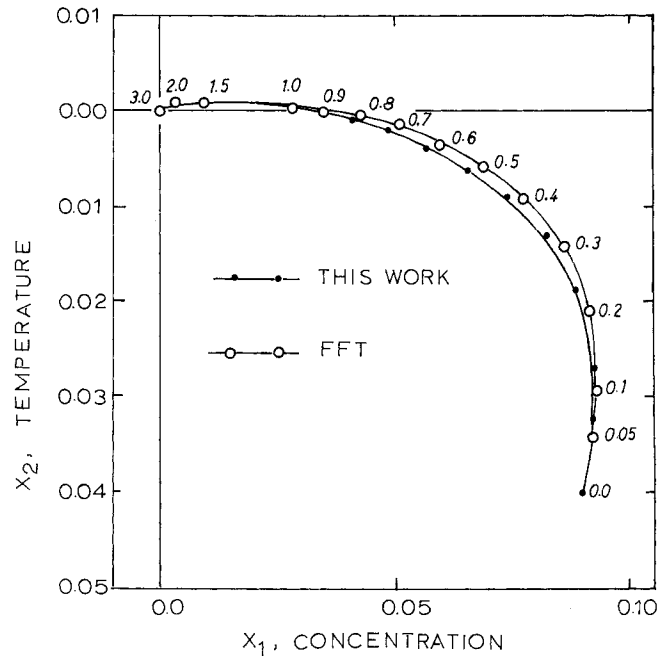

Fig. 3. State trajectory of proportional control CSTR, $k = 0.0$.

most reach the steady state when $t = 2$, so $t_f = 5$ is long compared to dynamic response time of the system. In such a case, if the initial control policy is not chosen properly, the controls will bring the states far away from the vicinity of the steady state; therefore, instability in the backward integration of the adjoint equations arises in the second variational method. Furthermore, the method is sensitive to the integration time step size. At $h = 0.1$, optimal solution can only be obtained when $k = 20.0$ where one stable equilibrium point exists, that is, one steady state. In order to obtain optimal performance index for comparison and to avoid instability in the backward integration of the adjoint equations, a smaller integration time step size of $h = 0.025$ is used and the system is optimized in two time sections. Except at $k = 20.0$, to ensure convergence with $t_f = 5$ with the use of second variation method, optimal control policy is first sought with $t_f = 2$ to yield the initial control policy for $0 \leq t < 2$ to be used for the longer time interval. For the rest of the time interval, that is, $2 \leq t < 5$, u is set at zero. This scheme for determining the initial control policy yielded the optimal control policy without any difficulty.

The nonlinear exothermic CSTR has been the center of interest for the comparison of optimization procedures. Since it was proposed by Aris and Amundson (1957), many interesting studies have been made on this system. Recently, existence of multiple solutions in the optimization of this system has been observed by Luus and Cormack (1972). Therefore, in this work two initial states are considered. They are $\mathbf{x}'(0) = (0.00\ 0.05)$ and $\mathbf{x}'(0) = (0.09\ 0.09)$. In each case the matrix $\mathbf{Q}$ is determined by Equation (14) with $\mathbf{x} = \mathbf{x}(0)$. The matrices for these two initial states are respectively

$$\mathbf{Q} = \begin{bmatrix} -0.0056 & -0.0399 \\ -0.0399 & -0.1795 \end{bmatrix} \tag{44}$$

$$\mathbf{Q} = \begin{bmatrix} -0.0046 & -0.0578 \\ -0.0578 & -0.1734 \end{bmatrix} \tag{45}$$

Results, together with those of Cormack and Luus (1972), are shown in Table 3. As seen from Figure 4, both trajectories obtained by the second variational

TABLE 3. PERFORMANCE INDICES FOR NONLINEAR CSTR

$h = 0.01$

Method	I	Percentage subop-timality	z^*	No. of iter-ations	Compu-tation time
		$\mathbf{x}(0) = \begin{pmatrix} 0.00 \\ 0.05 \end{pmatrix}$			
Optimal	0.02662			24	1.8
This work	0.02670	0.30	−121	5	0.4
C. and L.**	0.02662	0.00		20	1.2
		$\mathbf{x}(0) = \begin{pmatrix} 0.09 \\ 0.09 \end{pmatrix}$			
Optimal	0.1332			27	2.0
This work	0.1338	0.45	−118	9	0.6
C. and L.**	0.1334	0.15		25	1.7

** Cormack and Luus.

method and the suboptimal procedure of Cormack and Luus tend to go away from the origin (that is, steady state). This is attributed to the fact that the control policy obtained by the second variational method is final time dependent and so is the algorithm of Cormack and Luus, since both procedures involve integration of the adjoint equations. In the proposed method, the scalar adjoint is constant and the control policy is of feedback nature which corrects the deviation of the state from the steady state. Figure 5 shows the comparison of the control policies when $\mathbf{x}'(0) = (0.00\ 0.05)$. Even though a different trajectory is obtained by the proposed method, the suboptimal control policy follows closely to the optimal policy except at later stage when higher controls are used to force the states to the origin. In order to supplement the observation that the optimal trajectory obtained by the second variational method is final time dependent, a larger final time of $t_f = 3$ is investigated. In this case, Equation (14) is evaluated at $\mathbf{x} = \mathbf{0}$. The matrix $\mathbf{Q}$ is

$$\mathbf{Q} = \begin{bmatrix} -0.00377 & -0.03135 \\ -0.03135 & -0.19442 \end{bmatrix} \qquad (46)$$

With an optimizing $\hat{z}^*$ of -112.5, the suboptimal performance index is 0.02760 and the optimal one is 0.02754. With $t_f = 3$, both optimal and suboptimal control policies guide the states towards the origin as is shown in Figure 6.

The final example is the plug flow tubular reactor system. The transformation matrix $\mathbf{Q}$ is obtained from Equation (14) with $\mathbf{x} = \mathbf{x}(0)$ and is given by

$$\mathbf{Q} = \begin{bmatrix} -160.45 & 25.58 \\ 25.58 & -38.86 \end{bmatrix} \qquad (47)$$

The optimizing $\hat{z}^*$ is 0.8599. At an initially chosen control of $u(0) = 0.5$ atm. and $h = 0.08$, it takes 8 iterations and 0.5 second of computation time to obtain $x_2 = 0.01507$ by the proposed method, while the second variational method gives a maximum of $x_2 = 0.01508$ in 26 iterations and 2.3 seconds. The maximum obtained by Cormack and Luus is $x_2 = 0.01503$. The three control policies are compared in Figure 7 to emphasize the lack of sensitivity of x_2 on the control policy.

As has been pointed out, the determination of $\mathbf{Q}$ is an approximate one because $\hat{z}^*$ is not precisely known

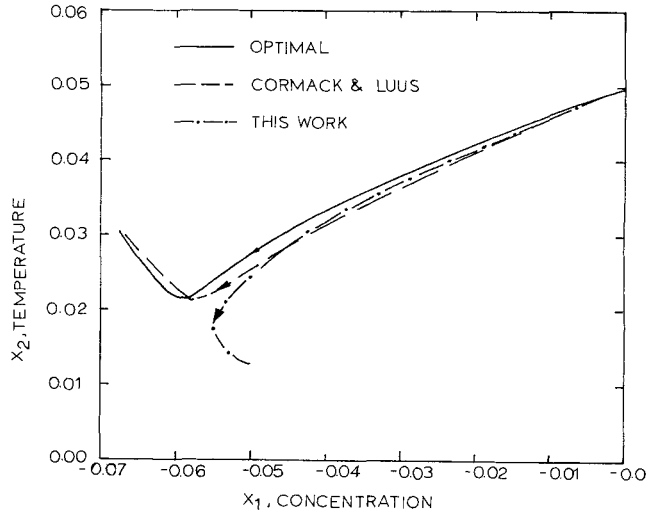

Fig. 4. State trajectory of nonlinear CSTR, $t_f = 0.78$.

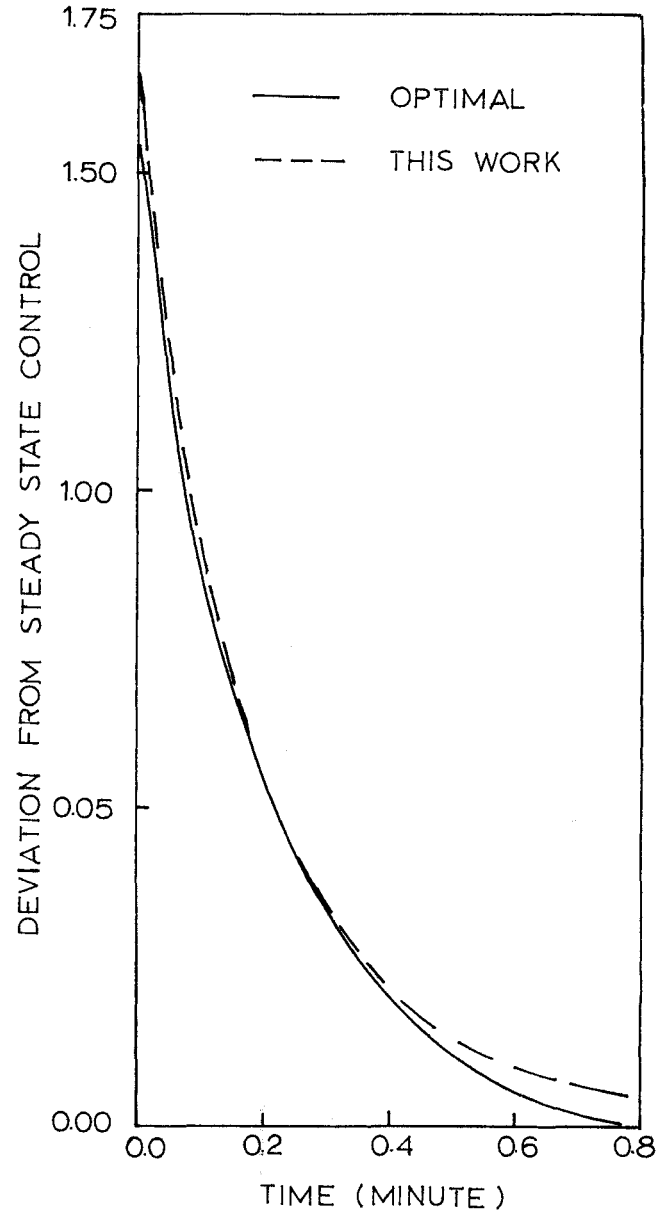

Fig. 5. Control policy for nonlinear CSTR, $t_f = 0.78$ and $x(0) = \begin{pmatrix} 0.00 \\ 0.05 \end{pmatrix}$.

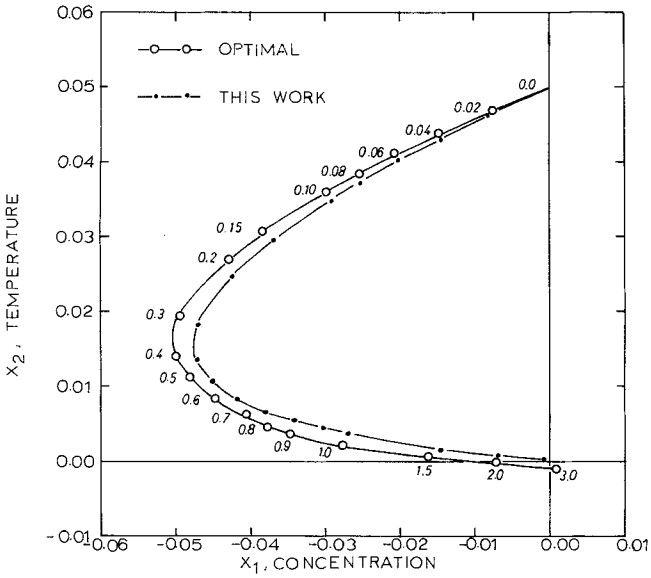

Fig. 6. State trajectory for nonlinear CSTR, $t_f = 3$.

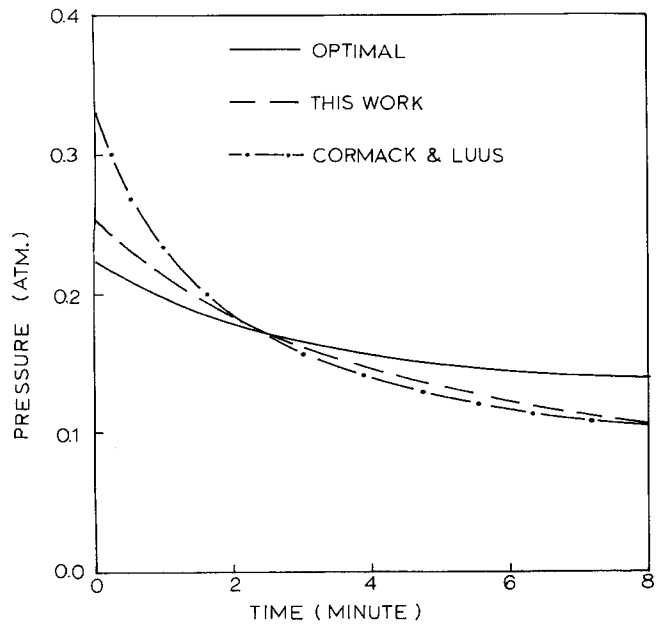

Fig. 7. Control policy for pressure control tubular reactor.

during the determination, and $\mathbf{x}$ and $\mathbf{u}$ in Equations (14) and (21) are taken at $\mathbf{x} = \mathbf{0}$ and $\mathbf{u} = \mathbf{0}$ or $\mathbf{x} = \mathbf{x}(0)$ and $\mathbf{u} = \mathbf{u}(0)$ instead of some state characteristic of the system. However, except in the case of the nonlinear exothermic CSTR, the optimizing adjoint parameters are of the order of unity. This supports that $\hat{z}$ set to unity in the determination of $\mathbf{Q}$ is applicable. In all cases, for the starting choice of $\hat{z}$, $\mathbf{u}(0)$ is obtained by solving $\mathbf{f}(\mathbf{x}(0), \mathbf{u}(0)) = \mathbf{0}$, and thus the proposed suboptimal procedure avoids the guessing of the initial control policy which is required for optimal solution by variational methods. No numerical instability arises in the proposed method and the number of iterations required to obtain the optimizing $\hat{z}^*$ is low. With the exception in the case of the tubular reactor where the performance index is not sensitive to the pressure control, the proposed suboptimal procedure yields a control policy close to the optimal one.

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NOTATION

$\mathbf{A}$ = state matrix
$\mathbf{B}$ = control matrix
c = constant
$\mathbf{f}$ = dynamic vector function
H = Hamiltonian
h = integration time step size
I = performance index
k_1, k_2 = constants in Equation (36)
k = proportional control constant for CSTR
$\mathbf{m}$ = vector
n = dimension of state vector
$\mathbf{Q}$ = transformation matrix
$\mathbf{R}$ = control weighting matrix
r = dimension of control vector
$\mathbf{S}$ = state weighting matrix
t = time
$\mathbf{u}$ = control vector
V = quadratic functional
$\mathbf{w}$ = vector, Equation (26)
$\mathbf{x}$ = state vector
$z, \hat{z}$ = adjoint variables

Greek Letters

φ = performance index integrand

Subscripts

1, 2, 3 = component index
f = final state
i = index

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