a pure catalyst which catalyzes the reaction $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$ only. The value of performance index, that is, the mole fraction of the substance C present in the mixture at the reactor exit at $t = 1$, with the pure bang-bang policy used is 0.047918. Although this policy is only a suboptimal one, it compares quite favorably with the optimal singular solution obtained by Jackson (1968), who gives a value of performance index of only 0.3% smaller, that is, 0.048065. Also, the computation time required for the present algorithm to obtain this bang-bang solution is only 6 s of CPU time on an IBM 370/155 computer with 250 integration steps. These results seem to suggest that the bang-bang catalyst blending should be used for most practical purposes for the present problem; since it can be implemented more easily than the singular one, it requires much less computation time, and it also has a fairly good degree of suboptimality.

In Figure 9, the change in the value of performance index with the number of iterations in applying algorithm to solve the present suboptimal bang-bang control problem is illustrated for two different initial control estimates, $u^o(t) = 1.0$ and $u^o(t) = 0.5$ for $0 \leq t \leq 1$. It is seen that the choice of the initial control policy has essentially no effect on the rapid convergence characteristics in using the proposed algorithm. For both choices of the initial control policy, the algorithm has been able to maximize the performance index to an almost optimal value within the first iteration. This confirms the same type of results observed in solving the preceding three linear lumped parameter systems.

In summary, for linear lumped parameter systems, these examples have shown that the proposed algorithm effectively solves in reasonably small computation time the singular and/or bang-bang control problems with high state dimensionality and multiple controls. From all numerical experience, the algorithm has a very rapid convergence characteristics, allows large changes in control variables in successive iterations, and gives fairly good suboptimal results without regard to the choice of the initial control policy. Although the exact switching times are not calculated by the algorithm, the large number of advantages of the algorithm illustrated in the preceding examples as well as in other nonlinear and distributed system examples presented in part II should definitely suggest that the proposed algorithm is a very effective suboptimal procedure for solving singular and/or bang-bang control problems.

Manuscript received November 26, 1975 and accepted January 29, 1976.

II. Applications to Nonlinear Lumped and Distributed Systems

A new and simple algorithm based on the piecewise maximization of the Hamiltonian and a limiting process utilizing a penalty function of the control variables for the computation of suboptimal singular and/or bang-bang control, previously developed and applied to linear lumped systems in Part I, is tested on four typical nonlinear lumped and distributed systems of particular chemical engineering interest. The computational results have shown that the proposed algorithm is a very effective method for solving singular and/or bang-bang control problems with high state dimensionality, extreme nonlinearity, and multiple controls.

SCOPE

In Part I, a new and simple algorithm for the computation of suboptimal singular and/or bang-bang control has been developed and applied successfully to several linear lumped parameter systems. The proposed algorithm is based on the piecewise maximization of the Hamiltonian and a limiting process utilizing a penalty function of the control variables. The algorithm has been shown to be very effective in solving large dimensional lumped parameter optimal control problems with multiple controls. It permits large changes in the control in the iterative control calculations with assured and rapid convergence characteristics regardless of the values of the initial control estimates. The computer implementation of the algorithm has also been shown to be very simple, requiring only a minimum amount of computer storage and computation time.

In this work, the effectiveness of the proposed algorithm in obtaining the suboptimal singular and/or bang-bang solutions of typical nonlinear lumped and distributed control problems is examined. The basic lumped parameter test problems are the optimal start-up or minimum-time control of an autothermic reaction system (Jackson, 1966), a two-stage continuous stirred-tank reactor (CSTR) system (Siebenthal and Aris, 1964; Edgar and Lapidus, 1972*b*; Luus, 1974*a*, 1974*b*), and a six-plate gas absorber with nonlinear gas-liquid equilibrium relationship (Lapidus and Luus, 1967; Weber and Lapidus, 1971). The determination of the optimal catalyst activity distribution policy in a distributed parameter, nonisothermal tubular reactor with radial heat and mass diffusion is also studied. These four test problems represent the typical chemical engineering optimal control problems with high state dimensionality, extreme nonlinearity, and multiple controls. The practical implications of the computational results are discussed, and the comparisons of the proposed algorithm with several existing techniques are given.

CONCLUSIONS AND SIGNIFICANCE

From examination of the numerical and graphical results for the chosen test problems presented in this paper, it can be concluded that the application of proposed algorithm based on the piecewise maximization of the Hamiltonian and a limiting process utilizing a penalty function of the control variables yields very acceptable, suboptimal singular and/or bang-bang control solutions with little expenditure of computer storage and computa-

tion time. In addition to the advantage of the algorithm in requiring no auxiliary linearization procedures or linearized approximate system models in solving the nonlinear lumped and distributed control problems, the computed results have shown that the algorithm has retained all the advantages previously demonstrated for linear lumped parameter control problems. Comparisons of the computed results for the selected test problems such as the two-stage CSTR system with other reported studies have also indicated that the present algorithm yields better performance than the differential dynamic programming and penalty function approach of Edgar and Lapidus (1972*b*), as well as the approach of direct search on the feedback gain matrix of Luus (1974*a*, 1974*b*).

Thus, the suboptimal singular and/or bang-bang control algorithm based on the piecewise maximization of the Hamiltonian and a limiting process utilizing a penalty function of control variables as presented in this work offers the advantages of effectiveness and simplicity, coupled with good performance, as is demonstrated.

SYSTEM EXAMPLES

In what follows, a number of different nonlinear lumped and distributed parameter systems which have been used to test the feasibility and efficiency of the piecewise Max-*H* and penalty function algorithm for suboptimal singular bang-bang control presented in Part I are briefly described. Most of these system examples are of direct chemical engineering interest, having high state dimensionality, extreme nonlinearity, and multiple controls.

Nonlinear, Lumped Parameter Systems

Optimal Start-up of an Autothermic Reaction System. The first nonlinear lumped parameter problem considered was to determine an optimal start-up procedure for an autothermic reaction system in which the first-order reversible reaction $A \rightleftarrows B$ is occurring. This problem was first presented by Jackson (1966) and is of some practical significance. Thus, it is known that certain exothermic reactions of considerable commercial importance, such as the ammonia synthesis reaction, make use of a regenerative heat exchanger between the reactant and product streams in such a way that the reaction system is thermally self-sustaining, or autothermic, when operating steadily. These types of reactions cannot be started up without supplying heat to the reactants from an external source such as a heat exchanger plus a reactant preheater, and normally the external heating may be withdrawn once the reaction mixture has been ignited. In the simplest type of autothermic reaction system as presented by Jackson (1966), the reactor is adiabatic, and its start-up and operation are controlled by regulating the external heat supply to the reactant preheater (denoted by u_1) and the fraction of the hot gas leaving the reactor which passes through the regenerative heat exchanger (denoted by u_2). The dynamical behavior of this autothermic reaction system can be represented by (Jackson, 1966)

$$\dot{x_1}(t) = R(x_1, x_2) - x_1 \tag{1}$$

$$\gamma \dot{x}_2(t) = u_1 - u_2(x_2 - x_{20}) + \alpha R(x_1, x_2) \tag{2}$$

where x_1 and x_2 are the mole fraction and temperature (°F) of the reactant A in the reactor, respectively. $R(x_1, x_2)$ is the reaction rate expression given by

$$R(x_1, x_2) = k_1(x_2)\,[1 - x_1] - k_2(x_2)x_1$$

$$k_1(x_2) = 2\,417 \exp\,[-5\,000/x_2]$$

$$k_2(x_2) = 2.683 \times 10^5 \exp\,[-10\,000/x_2]$$

The parameter γ is the ratio of the thermal capacity of reactant vs. the specific heat of reaction mixture on a molar basis, x_{20} is the temperature (°F) of the reactant A at entry to the cold side of the exchanger, and α is the adiabatic temperature rise (°F) of the reaction. The values of these parameters are

$$\gamma = 1 \qquad x_{20} = 300 \qquad \alpha = 500$$

Also, physical considerations require the control variables $u_1(t)$ and $u_2(t)$ to be bounded by

$$0 \leq u_1(t) \leq 200 \tag{3}$$

$$0 \leq u_2(t) \leq 1.0 \tag{4}$$

The start-up problem is then to find the optimal control variables $u_1(t)$ and $u_2(t)$ which will transfer the autothermic reaction system from the initial operating conditions with the mole fraction and temperature of component A in the feed, $x_1(0) = 0.0$ and $x_2(0) = 300$°F, respectively, to the desired final steady state operating conditions with $x_1(t_f) = 0.7$ and $x_2(t_f) = 800$°F in a minimum time t_f. The optimum start-up procedure to be obtained will dictate a suitable compromise between the desirability of reaching steady state operating conditions quickly and the cost of the external heating thus required. Jackson (1966) has solved this problem using the maximum principle. His solution will be compared with the present work.

Optimum Start-Up of Two-Stage Continuous Stirred-Tank Reactor (CSTR) *System.* The second nonlinear lumped parameter system problem considered was to determine the optimum start-up procedure for a two-stage CSTR in series with heating and cooling controllers. The system model used was first suggested by Siebenthal and Aris (1964) and recently studied by Edgar and Lapidus (1972*b*) and by Luus (1974*a*, 1974*b*). It represents a typical system of high state dimensionality, extreme nonlinearity, and multiple controls of direct chemical engineering interest. In a dimensionless, normalized form, the governing equations are a set of highly nonlinear ordinary differential equations which can be written in a vector form as

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}, t) \tag{5}$$

where $\mathbf{x}$ is a four-dimensional vector with the components x_1 and x_3 denoting the normalized concentration variables and x_2 and x_4 representing the normalized temperature variables. The components of $\mathbf{u}$, that is, u_1 and u_2, are two normalized control variables having cooling capacity only. The specific form of (5) along with the numerical values of the parameters can be found as Equations (7) to (14) in the paper of Edgar and Lapidus (1972*b*). It is assumed that both reactors are initially at the steady state temperature of the second reactor, and the start-up problem is to find the optimal control variables $u_1(t)$ and $u_2(t)$ for the two reactors to reach in a minimum time t_f, some final steady state compositions and temperatures where the reaction rate is maximized with respect to the operating conditions. A set of suitable initial and final operating conditions for this start-up problem can be taken as (Edgar and Lapidus, 1972*b*)

$$\mathbf{x}(0) = [0.1962 \quad -0.0372 \quad 0.0946 \quad 0]^T \tag{6}$$

$$\mathbf{x}(t_f) = [0 \quad 0 \quad 0 \quad 0]^T \tag{7}$$

Also, the normalized control variables are bounded by

$$-8.1558 \leq u_1(t) \leq 8.1558 \tag{8}$$

$$-3.4385 \leq u_2(t) \leq 3.4385 \tag{9}$$

The solution to this time optimal control problem has been shown to be of a combined singular bang-bang type by Siebenthal and Aris (1964) qualitatively and by Edgar and Lapidus (1972*b*) quantitatively. The latter authors employed first an analytical apparent linearization by the method of Pearson (1962) which converts (5) to an approximate linear model in the vector form

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}, \mathbf{u}, t) = \mathbf{A}(\mathbf{x}, \mathbf{u}, t) \cdot \mathbf{x} + \mathbf{B}(\mathbf{x}, \mathbf{u}, t) \cdot \mathbf{u} \tag{10}$$

An approach using the discrete dynamic programming with penalty functions (DDP-PF) was then used to handle the control and final state variable constraints and to solve the singular and/or bang-bang control problem as a limit of a series of nonsingular and/or bang-bang problems. Recently, another approach using the direct search of the feedback gain matrix based on a linearized form of (5) for obtaining the time suboptimal control of the same two-stage CSTR problem was given by Luus (1974*a*, 1974*b*). The results of both previous studies will be compared with this work.

Time Optimal Control of a Six-Plate Nonlinear Gas Absorber System. The final nonlinear lumped parameter system investigated was a six-plate gas absorber system with a nonlinear liquid-vapor equilibrium relationship controlled by the inlet fed streams as detailed by Lapidus and Luus (1967). This nonlinear system with six state and two control variables can be modeled by the normalized system equation in the vector form of (5). Here, $x_i(t)$ $(i = 1, 2, \ldots 6)$ is the liquid composition leaving the i^{th} plate (pound solute per pound absorbent), and the control variables $u_1(t)$ and $u_2(t)$ are the inlet liquid and vapor compositions at the first plate and the sixth plate, respectively. The specific form of (5), its initial condition, and the corresponding values of parameters can be found as Equations (42) to (44) in the work of Weber and Lapidus (1971). The constraints on the control variables are (Weber and Lapidus, 1971)

$$0.0 \leq u_1(t) \leq 0.045 \tag{11}$$

$$-0.025 \leq u_2(t) \leq 0.080 \tag{12}$$

The problem is to find the control variables $u_1(t)$ and $u_2(t)$ satisfying the constraint which will drive the state vector $\mathbf{x}$ from its initial state $\mathbf{x}(0)$ to the desired state, the origin $\mathbf{x} = \mathbf{0}$, in a minimum time t_f. The linear version of this time optimal control problem has been solved in a number of previous works, for example, by Lesser and Lapidus (1966), Chant and Luus (1968), Bennett and Luus (1971), Bashien (1971), Schlossmacher (1973), and Luus (1974*c*). The present work, however, is concerned with the solution of the same problem with a nonlinear vapor-liquid equilibrium relationship.

Nonlinear Distributed Parameter Systems

The present computational algorithm has been extended to obtain the suboptimal control for a number of linear and nonlinear distributed parameter systems, and the results will be reported separately. The effectiveness of the algorithm in solving the singular and/or bang-bang control problems, however, can be illustrated by determining the optimal catalyst activity distribution policy in a radially dispersed, tubular reactor in which a catalytic consecutive reaction occurs under nonisothermal conditions. In the present work, two types of consecutive reactions have been considered. One is the irreversible reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ and the other the reversible reaction $A \underset{k_3}{\overset{k_1}{\rightleftarrows}} B \xrightarrow{k_2} C$, where A is the raw material, B the desired product, and C the undesired by-product. By denoting the dimensionless axial reactor length as t and the dimensionless radial coordinate as r, the dimensionless concentrations of components A and B, $x_1(t, r)$, and $x_2(t, r)$, respectively, as well as the dimensionless reactor temperature $x_3(t, r)$, can be described by the following set of nonlinear partial differential equations:

$$\frac{\partial x_1}{\partial t} = 0.48 \left[\frac{\partial x_1^2}{\partial r^2} + \frac{1}{r} \frac{\partial x_1}{\partial r} \right] + 0.5\, w(t, r) R_1(x_1, x_2, x_3) \tag{13}$$

$$\frac{\partial x_2}{\partial t} = 0.48 \left[\frac{\partial x_2^2}{\partial r^2} + \frac{1}{r} \frac{\partial x_2}{\partial r} \right] + 0.5\, w(t, r) R_2(x_1, x_2, x_3) \tag{14}$$

$$\frac{\partial x_3}{\partial t} = 0.67 \left[\frac{\partial x_3^2}{\partial r^2} + \frac{1}{r} \frac{\partial x_3}{\partial r} \right] + w(t, r) [0.2\, R_1(x_1, x_2, x_3) + 0.05\, R_2(x_1, x_2, x_3)] \tag{15}$$

Here, a specific set of values of the radial Peclet numbers for heat and mass transfer and the first and third Damköhler numbers have been included in Equations (13) to (15). $w(t, r)$ is the catalyst activity distribution function with its value between zero and one. For the irreversible reaction system, the dimensionless reaction rate expressions R_1 and R_2 are given by

$$R_1(x_1, x_2, x_3) = -0.5 \times 10^9\, E_1 \cdot x_1 \tag{16}$$

$$R_2(x_1, x_2, x_3) = 0.5 \times 10^9\, E_1 \cdot x_1 - 0.8 \times 10^{15}\, E_2 \cdot x_2 \tag{17}$$

and for the reversible reaction system

$$R_1(x_1, x_2, x_3) = 0.3 \times 10^{12}\, E_3 \cdot x_2 - 0.5 \times 10^9\, E_1 \cdot x_1 \tag{18}$$

$$R_2(x_1, x_2, x_3) = 0.5 \times 10^9\, E_1 \cdot x_1 - 0.3 \times 10^{12}\, E_3 \cdot x_2 + 0.6 \times 10^{13}\, E_2 \cdot x_2 \tag{19}$$

where

$$E_1 = \exp[-19.35/x_3], \quad E_2 = \exp[-30.0/x_3], \quad E_3 = \exp[-35.0/x_3]$$

The initial and boundary conditions for (18) and (19) are

$$x_1(0, r) = 1.0, \quad x_2(0, r) = 0.0, \quad x_3(0, r) = 1.0 \tag{20}$$

$$\partial x_1(t, 0)/\partial r = \partial x_2(t, 0)/\partial r = \partial x_3(t, 0)/\partial r = 0 \tag{21}$$

$$\partial x_1(t, 1)/\partial r = \partial x_2(t, 1)/\partial r = 0, \quad \partial x_3(t, 1)/\partial r = -Q \tag{22}$$

where Q is the dimensionless wall heat flux. The optimal design problem is to choose the best distributed catalyst activity function $w(t, r)$ subject to bounds

$$0 \leq w(t, r) \leq 1 \quad \text{for} \quad 0 \leq t \leq 1, \quad 0 \leq r \leq 1 \tag{23}$$

so as to maximize the dimensionless area-averaged concentration of the desired product B in the reactor effluent

$$J = \bar{x}_2(1) = 2 \int_0^1 r x_2(t, r)\, dr \tag{24}$$

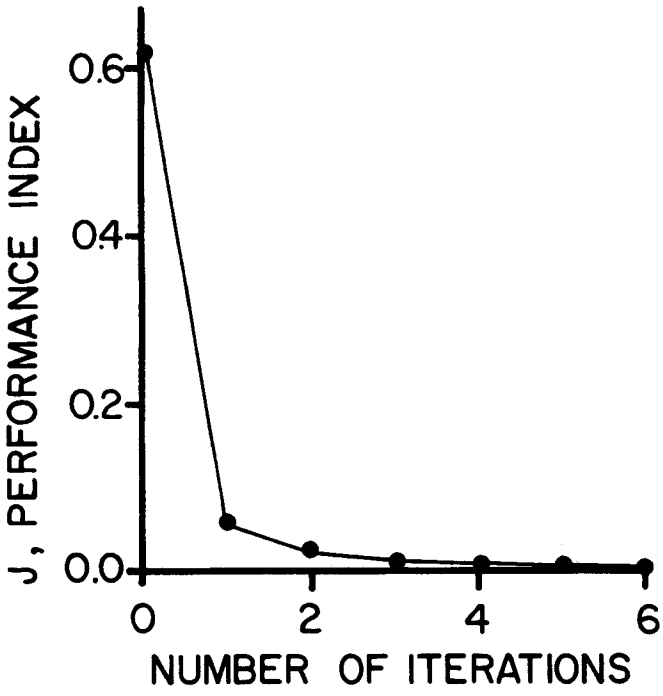

Fig. 1. Performance index versus number of iterations for the start-up of the autothermic reaction system.

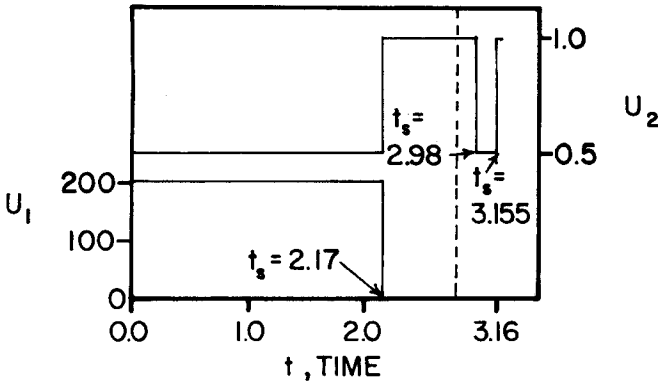

Fig. 2. Computed combined bang-bang ($0 \leq t \leq 2.8$) and singular bang-bang ($2.8 < t \leq t_f$) control policy for the start-up of the autothermic reaction system.

It may be mentioned that although a related second-order distributed parameter optimization problem in determining the optimal dimensionless wall heat flux $Q(t)$ has been described in some recent studies such as Denn et al. (1966) and Seinfeld and Lapidus (1968*a*), the present third-order system example seems to be one of the highest-order, nonlinear distributed parameter reactor optimization problems that have ever been considered in the chemical engineering literature.

NUMERICAL RESULTS

Nonlinear Lumped Parameter Systems

Optimal Start-up of an Autothermic Reaction System. The present algorithm has been applied to compute a suboptimal bang-bang control which moves the autothermic reaction system, Equations (1) and (2), as closely as possible to the desired steady state operating conditions in minimum time. The results calculated based on a series of assumed final time t_f by using a weighting matrix $\mathbf{Q} = \text{diag}\,[1.0,\ 10^{-6}]$ and initial control estimates $u_1^0(t) = 100$, $u_2^0(t) = 0.75$ for $0 \leq t \leq t_f$ are summarized as follows:

Fixed final time t_f	$x_1(t_f)$	$x_2(t_f)$	Performance index $J = \mathbf{x}^T(t_f)\,\mathbf{Q}\,\mathbf{x}(t_f)$
2.4	0.6687	820.70	0.1407×10^{-2}
2.8	0.6946	806.90	0.7662×10^{-4}
3.0	0.6953	804.50	0.3836×10^{-4}
3.2	0.6953	804.80	0.3868×10^{-4}

The results of a phase plane analysis by Jackson (1966) for this problem have shown that a pure bang-bang control will not be able to drive this reaction system to the desired steady state operating condition with $x_1(t_f) = 0.70$ and $x_2(t_f) = 800°\text{F}$. The above calculations with different values of final time seem to confirm this analysis. Taking the value of $t_f = 2.8$ as the minimum time, the computation time required for obtaining this bang-bang control strategy with 400 integration steps between $t = 0$ and $t = t_f$ is 15 s of CPU time on an IBM 370/155 computer. Figure 1 illustrates the performance index as a function of the number of iterations for this case.

To drive the reaction system to the desired steady state, a combined suboptimal control which consists of a pure bang-bang control for $0 \leq t \leq 2.8$ followed by a singular bang-bang control for $2.8 < t \leq t_f$ has been calculated by the algorithm as shown in Figure 2. This computation uses a weighting matrix $\mathbf{Q} = \text{diag}\,[1.0,\ 10^{-3}]$ and gives a minimum final time $t_f = 3.16 = 2.8$ (pure bang-bang) $+ 0.36$ (singular bang-bang). The final state values are $x_1(t_f) = 0.6990$ and $x_2(t_f) = 799.86$. As seen in Figure 2, u_2 is of a pure bang-bang type for $2.98 \leq t \leq 3.155$, while u_1 has a singular arc for the same time period with its value being very close to zero. The last result suggests that it may be simpler to control this reaction system by fixing $u_1(t) = 0.0$, and by applying a pure bang-bang control for $u_2(t)$ for $2.8 \leq t \leq t_f$. The final minimum time for this control policy computed by the algorithm is $t_f = 3.175$, requiring only another 0.0375 operation time to drive the state from $\mathbf{x}^T(2.8) = [0.6946,\ 806.90]^T$ to $\mathbf{x}^T(3.175) = [0.6990,\ 800.14]^T$. Further calculations by the algorithm have shown that an additional operation time of only 0.54 is required to drive x_1 from 0.6990 to 0.700. This corresponds to a total operation time of 3.715. For this reaction system, Jackson (1966) has suggested

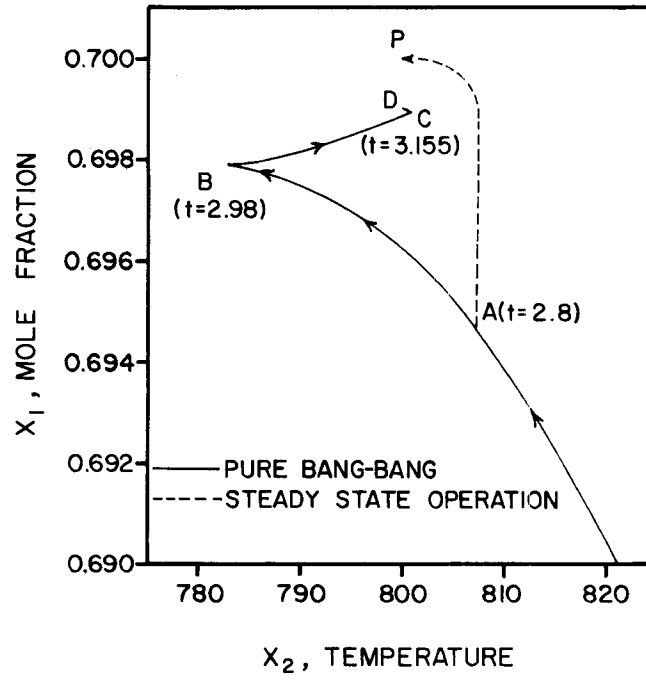

Fig. 3. Computed phase plane for the start-up of the autothermic reaction system.

qualitatively that its desired steady state can be reached very simply by applying the maximum possible heating control with an initial bang-bang control of $u_1 = 200$ and $u_2 = 0.5$, and switching later to the values $u_1 = u_{1s} = 0.0$ and $u_2 = u_{2s} = 0.7$ required for steady state operation in the specified final state. However, quantitative calculations of this combined bang-bang steady state control by the algorithm have shown that an additional steady state operation time of 3.15 after the initial bang-bang control period $0 \leq t \leq 2.8$ is required to assure $0.7000 \geq x_1(t_f) \geq 0.6997$ and $800.0 \leq x_2(t_f) \leq 801.0$. This corresponds to a total operation time $t_f = 5.95$, which is much larger than the results obtained by applying an initial pure bang-bang control ($0 \leq t \leq 2.8$) followed by either a singular bang-bang control ($t_f = 3.160$) or a pure bang-bang control of $u_2(t)$ only ($t_f = 3.1750$). This is further illustrated in Figure 3, where the state trajectories of these procedures are shown. The point A represents the final state resulted from the initial pure bang-bang control during the time period $0 \leq t \leq 2.8$. After this point, the path ABCD corresponds to the case of a pure bang-bang control of $u_2(t)$ only, while the path AP represents the steady state operation suggested by Jackson (1966). Although the state D is not sufficiently close to the desired steady state P, the operation time required to bring the reaction system from D to P is only 0.54. Thus, the overall control strategy shown by the path ABCDP represents a saving of operation time of 2.135 as compared to the path AP. Further illustrations of the applicability of the present algorithm in exploring the relative merits of different controls of several other chemical engineering systems are given as follows.

Optimum Start-up of a Two Stage CSTR System. The proposed algorithm has been applied to compare four types of control policy which will drive the two-stage CSTR system, Equation (5), from the initial state $\mathbf{x}(0)$, Equation (6), to the desired final state $\mathbf{x}(t_f) = 0$ in a minimum time t_f subject to the constraints, Equations (8) and (9). These include a pure bang-bang control, a combined singular bang-bang control, an initial bang-bang control followed by a singular control, and an initial bang-bang control followed by a steady-state control.

In Table 1, the computed values of performance indexes and final states with a pure bang-bang control for a series of final states are shown. Here, a quadratic performance index $J = \mathbf{x}^T(t_f)\ \mathbf{Q}\ \mathbf{x}(t_f)$ has been used. A minimum time of $t_f = 0.260$ seems to give the best performance index, $J = 0.3037 \times 10^{-4}$, with a pure bang-bang control, and the resulting state trajectories are shown in the upper part of Figure 4. As can be seen from this figure and Table 1, a disadvantage of the pure bang-bang control is that the final states are not sufficiently close to the origin. One reason for this disadvantage can be learned from the computed combined singular bang-bang control and state trajectories shown in Figure 5 and the lower part of Figure 4. The solid curves in Figure 5 represent the control policy calculated by the present algorithm, while the dashed curves in Figure 5 are

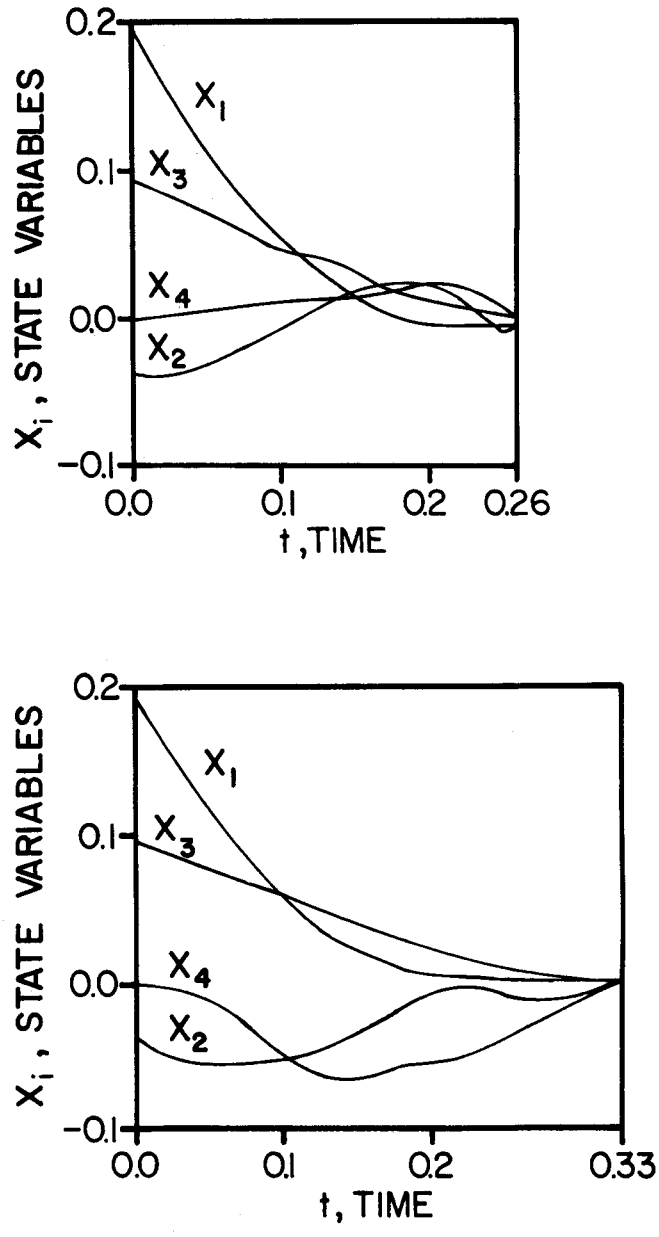

Fig. 4. Computed state trajectories for the two-stage CSTR system: (a) top: with pure bang-bang control (b) bottom: with combined singular bang-bang control.

the corresponding results obtained by Edgar and Lapidus (1972*b*). Note that in Figure 5 the unsaturated behavior of u_1 is an indication of possible singular control; the nearly saturated state of u_2 indicates probable bang-bang control. This fact thus explains why the preceding pure bang-bang control for both u_1 and u_2 fails to drive the final states sufficiently close to the origin. By using a weighting matrix $\mathbf{Q} = \text{diag}\ [1,1,1,1]$ in the quadratic performance index $J = \mathbf{x}^T(t_f)\mathbf{Q}\mathbf{x}(t_f)$ augmented with a control penalty $\epsilon \int_0^{t_f} \mathbf{u}^T\mathbf{u}\,dt$, where the

Table 1. Computed Results for the Minimum Time Start-up Control of the Two-Stage CSTR System: Pure Bang-Bang Control

Final time t_f	Performance index	$x_1(t_f)$	$x_2(t_f)$	$x_3(t_f)$	$x_4(t_f)$
0.20	0.2020×10^{-3}	−0.00180	0.00108	0.01341	0.00421
0.22	0.1034×10^{-3}	−0.00257	−0.00220	0.00899	0.00336
0.24	0.4809×10^{-4}	−0.00357	−0.00180	0.00523	0.00216
0.26	0.3037×10^{-4}	−0 00378	−0.00086	0.00350	0.00177
0.28	0.4151×10^{-4}	−0.00570	−0 00163	0.00230	0.00107
0.30	0.5181×10^{-4}	−0.00161	0.00193	0.00202	−0.00055

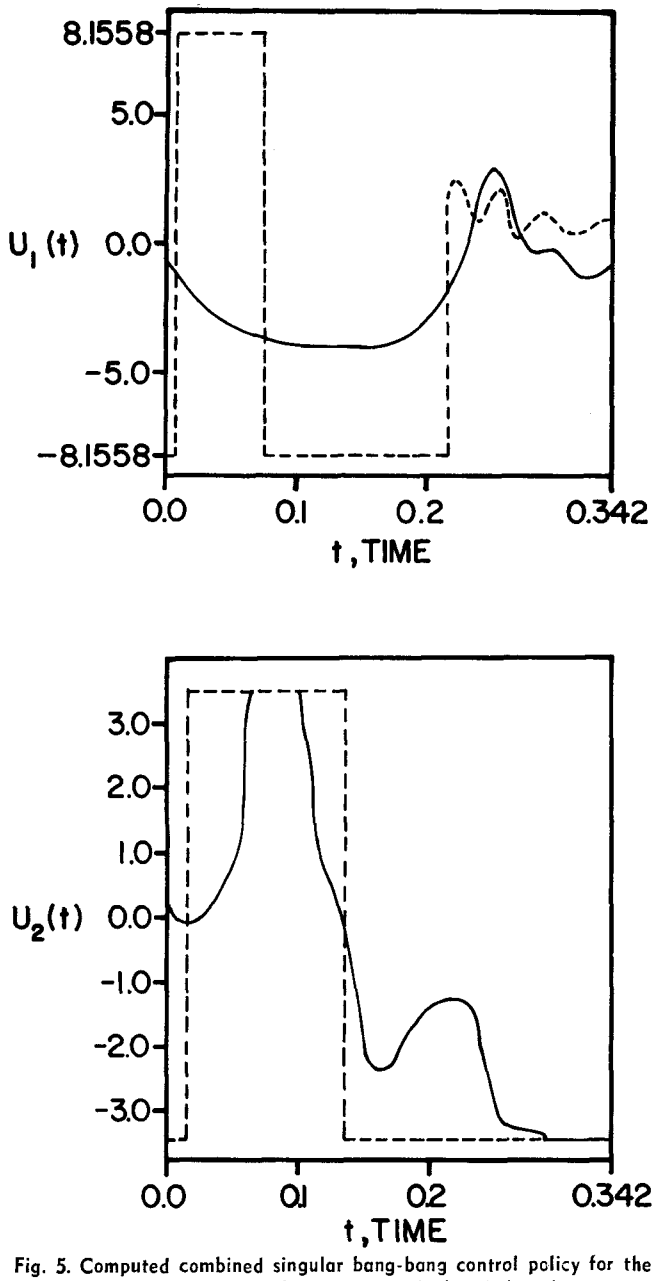

Fig. 5. Computed combined singular bang-bang control policy for the two-stage CSTR system: solid curves—calculated by the present algorithm; dashed curves—calculated by Edgar and Lapidus (1972*b*).

variable weighting coefficient $\epsilon = 10^{-5}$, the computed augmented performance index is $J_c = 0.9996 \times 10^{-5}$ with a minimum time $t_f = 0.330$ and the corresponding final states $\mathbf{x}^T(t_f) = [-0.00091, -0.00035, 0.00219, -0.00205]^T$. Although this performance index (0.9996×10^{-5}) is about 1.5% larger than the optimal value (0.9799×10^{-5}) obtained by Edgar and Lapidus, the smaller final time $t_f = 0.330$ calculated by the present algorithm seems to compare favorably with the result of Edgar and Lapidus, that is, $t_f = 0.342$. Furthermore, except for the final values of $x_3(t_f)$ and $x_4(t_f)$, the preceding final states $\mathbf{x}^T(t_f) = [-0.00091, -0.00035, 0.00219, -0.00205]^T$ are much closer to the origin than those calculated by Edgar and Lapidus, namely, $\mathbf{x}^T(t_f) = [-0.00171, 0.00103, 0.00173, -0.00169]^T$. Next, in order to compare more properly the results of both studies, the present algorithm was applied to obtain a combined singular bang-bang control at the fixed final time $t_f = 0.342$. By using the initial control estimates $u_1^0(t) = u_2^0(t) = 0.0$ for $0 \leq t \leq 0.342$ and an identity weighting matrix $\mathbf{Q} = \mathbf{I}$, the computed performance index is $J_c = 0.5405 \times 10^{-5}$, which is now much smaller than the value $J_c = 0.9799 \times 10^{-5}$ obtained by Edgar and Lapidus. The corresponding final states are also much closer to the origin for all four state variables than the results of Edgar and Lapidus, namely, $\mathbf{x}^T(t_f) = [-0.00094, -0.00021, 0.00136, -0.00162]^T$ vs. $\mathbf{x}^T(t_f) = [-0.00171, 0.00103, 0.00173, -0.00169]^T$.

It is worthwhile to comment briefly on some further comparisons of the present algorithm with the work of Edgar and Lapidus. For this nonlinear, two-stage CSTR system, Edgar and Lapidus employed first an analytical, apparent linearization by the method of Pearson (1962) which converted Equation (5) to an approximate, linear equation in the form of Equation (10). An approach based on the discrete dynamic programming with penalty functions (DDP-PF) was then used to handle the end point and control constraints and to solve the singular and/or bang-bang problem as a limit of a series of nonsingular and/or nonbang-bang problems. The latter limiting approach has also been used in the present algorithm. However, an inherent difficulty with the Pearson linearization procedure is that the algebraic efforts in obtaining the analytical expressions for the matrices $\mathbf{A}(\mathbf{x}, \mathbf{u}, t)$ and $\mathbf{B}(\mathbf{x}, \mathbf{u}, t)$ in Equation (10) will be too complex for higher-order systems, which also dictates a careful analytic work prior to numerical solution. For the present highly nonlinear, two-stage CSTR system, the linearized system matrices $\mathbf{A}(\mathbf{x}, \mathbf{u}, t)$ and $\mathbf{B}(\mathbf{x}, \mathbf{u}, t)$ are also quite sensitive to the assumed nominal state trajectories. For example, it was reported by Edgar and Lapidus that for all final times $t_f > 0.356$, the convergence to the original state equation by the Pearson linearization approach was difficult to attain without excessive amounts of computation time. In contrast, the present algorithm requires no auxiliary linearization procedures, and for all the system examples considered in this work, it has always been able to achieve stable and rapid convergence to the desired solutions with almost any initial control estimates and a reasonably small amount of computation time. For the combined singular bang-bang control of the two-stage CSTR system with a minimum time of $t_f = 0.342$, the present algorithm requires a CPU time of about 3 min on an IBM 370/155 computer. This compares favorably with the computation time of 4 min reported by Edgar and Lapidus using an IBM 360/91 computer. Finally, the current algorithm has a significant advantage in eliminating completely all the computer calculations and storage of auxiliary variables or functions such as H_u, $H_{u\lambda}$, H_{uu}, H_{ux}, etc., required in the control correction schemes of many first- and second-order methods for optimal control computation. In fact, the proposed algorithm requires the storage of the computed state variables only. As such, this new algorithm should compare favorably and complement significantly several existing effective algorithms for the solution of the singular and/or bang-bang control problems presented by Lapidus and his co-workers (Edgar and Lapidus, 1972*a*, 1972*b*; Schlossmacher and Lapidus, 1971; Seinfeld and Lapidus, 1968; Lapidus and Luus, 1967; Lesser and Lapidus, 1966; Grethlein and Lapidus, 1963) as well as by others.

The proposed algorithm was also applied to compute two other types of control policy. For an initial pure bang-bang control in the time period $0 \leq t \leq 0.260$ followed by a singular control for $t > 0.260$, the computed performance index is less than 10^{-5} (that is, $J_c = 0.9191 \times 10^{-5}$) at a final time of $t_f = 0.305$. If this pure bang-bang control is followed by a steady state control with $u_1(t) = u_2(t) = 0$ for $t > 0.260$, the computed final time for $J_c < 10^{-5}$ is $t_f = 0.307$, with $J_c = 0.9890 \times 10^{-5}$ These

Table 2. Comparison of Computed Values of Final Time and Performance Index for Different Types of Control Policy for the Two-Stage CSTR System

Control policy	Final time, t_f	Performance index, J_c
(1) Pure bang-bang control	0.260	0.3037×10^{-4}
(2) Combined singular bang-bang control	0.330	0.9996×10^{-5}
	0.342	0.5405×10^{-5}
(3) Combined singular bang-bang control by Edgar and Lapidus (1972*b*)	0.342	0.9799×10^{-5}
(4) Pure bang-bang ($0 \leq t \leq 0.260$) and singular control ($t > 0.262$)	0.305	0.9191×10^{-5}
(5) Pure bang-bang ($0 \leq t \leq 0.262$) and steady state control ($t > 0.260$)	0.307	0.9890×10^{-5}
(6) Suboptimal feedback and minimum-time control by Luus (1974*a*)	0.370	$\lvert x_i \rvert < 10^{-4}$
(7) Suboptimal feedback and minimum time control by Luus (1974*b*)	0.325	$\lvert x_i \rvert < 10^{-3}$

results along with those reported by others are summarized in Table 2.

The results on the suboptimal feedback and minimum time control by Luus (1974*a*, 1974*b*) included in Table 2 were obtained by a direct search procedure to find the best values for the elements in the feedback gain matrix so as to minimize the final time. It is seen in this table that for smaller values of performance index, say, $J_c < 10^{-5}$, the required final times computed by the present algorithm seem to compare favorably with the results of Luus. One significant advantage of the present algorithm is that its applicability is essentially independent of the choice of initial control estimates. In contrast, in applying the method of direct search of Luus, it is necessary to carry out some preliminary runs to determine the proper initial estimates of the elements of the feedback gain matrix and initial ranges for the random numbers in the search routine. In general, the computation time requirement of this direct search approach is greater than that required with the present control vector iteration procedure with a quadratic performance index such as $J = \mathbf{x}^T(t_f)\ \mathbf{Q}\mathbf{x}(t_f)$ used. Furthermore, the multidimensional optimization problem associated with the direct search method when applied to systems with high state dimensionality and multiple controls may present some computational difficulties. For example, the state equations must be integrated a large number of times at each iteration, and many iterations may be required to yield a control policy of high degree of suboptimality. Further comparisons of the direct search procedure and the current algorithm are discussed in the subsequent sections.

Time Optimal Control of a Six-Plate Nonlinear Gas Absorber System. This system example with six state and two control provides an ultimate test of the present algorithm in solving typical chemical engineering problems with high state dimensionality, extreme nonlinearity, and multiple controls. By solving this problem as a sequence of fixed final time problems with a weighting matrix $\mathbf{Q} = \mathbf{I}$ used in the quadratic performance index $J = \mathbf{x}^T(t_f)\ \mathbf{Q}\mathbf{x}^T(t_f)$, a final time of $t_f = 22.0$ was found to give the minimum performance index value of $J = 0.1778 \times 10^{-4}$ and the final state values of $\mathbf{x}^T(t_f) = [0.0023, 0.0013, -0.0014, -0.0026, 0.0001, 0.0012]^T$ with a pure bang-bang control. Although the final values of state variables are almost close to the origin, this bang-bang control seems to be unacceptable for real process operation be-

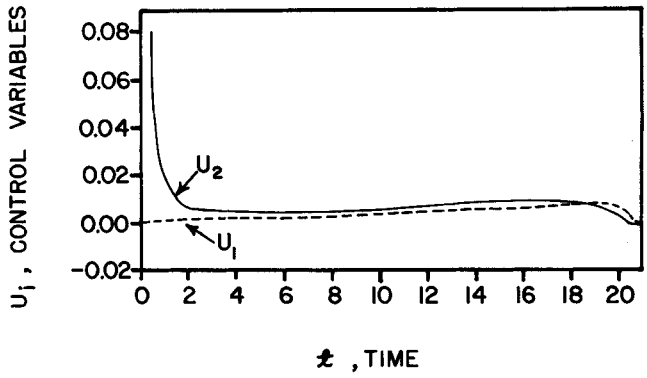

Fig. 6. Computed control trajectories for the six-plate nonlinear gas absorber system.

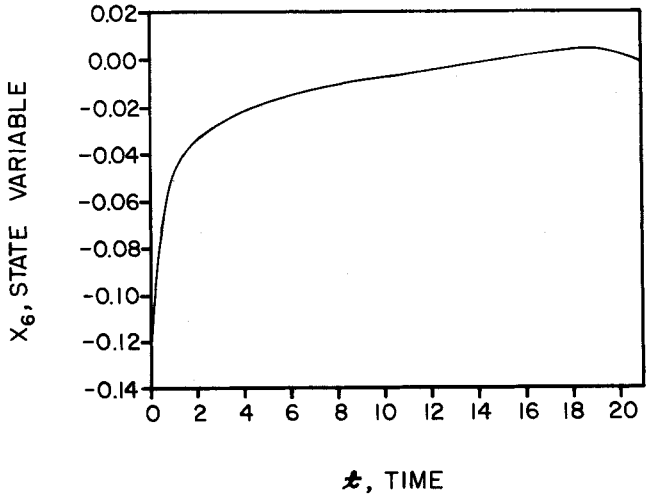

Fig. 7. Computed state variable x_6 for the six-plate nonlinear gas absorber system.

cause of the large number of switches on control variables resulted. Next, the algorithm was applied to compute the singular bang-bang control by augmenting the quadratic performance index $J = \mathbf{x}^T(t_f)\ \mathbf{x}(t_f)$ with a control penalty term $\epsilon \int_0^{t_f} \mathbf{u}^T\mathbf{u}\, dt$. For a final time of $t_f = 21.0$, the augmented performance index was found to be less than 10^{-5}, that is, $J_c = 0.9135 \times 10^{-5}$, when the variable weighting coefficient $\epsilon = 10^{-5}$. The corresponding values of state variables are $x^T(t_f) = [0.0003, -0.0015, -0.0022, -0.0012, 0.0001, -0.0000]^T$. The computation time required for obtaining this singular bang-bang control solution by using 400 integration steps between $t = 0$ and $t = t_f$ is 700 s of CPU time on an IBM 370/155 computer. Figure 6 shows the trajectories of both control variables $u_1(t)$ and $u_2(t)$ for this case. The highly singular nature of these control policies shown in the figure seems to explain the large number of switches on control variables of the preceding pure bang-bang control solution for the same problem. The state trajectory of one typical state variable x_6 is shown in Figure 7. Note that the above calculations were performed by an arbitrary set of initial control estimates, namely, $u_1^o(t) = u_2^o(t) = 0$ for $0 \leq t \leq t_f$. The stable and rapid convergence characteristics were always observed in all iterative calculations.

Nonlinear Distributed Parameter Systems

For both the reversible and irreversible consecutive reactions, $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B \xrightarrow{k_3} C$ and $A \xrightarrow{k_1} B \xrightarrow{k_2} C$, respectively, occurring in a radially dispersed packed-bed reactor modeled by Equations (13) to (15), the algorithm has been ap-

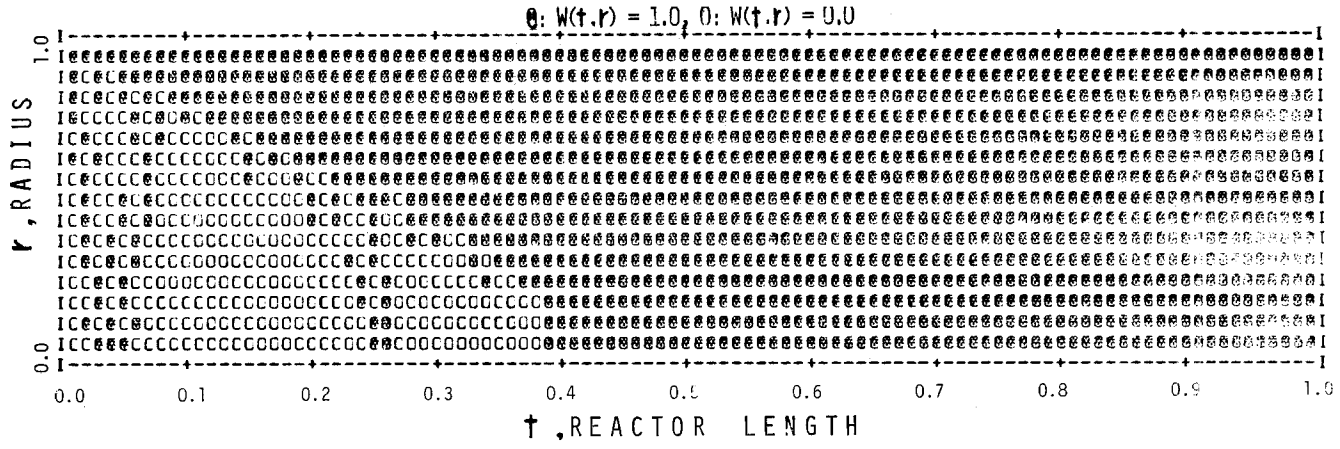

Fig. 8. Computed pure bang-bang type of catalyst activity distribution for the reaction A→B→C.

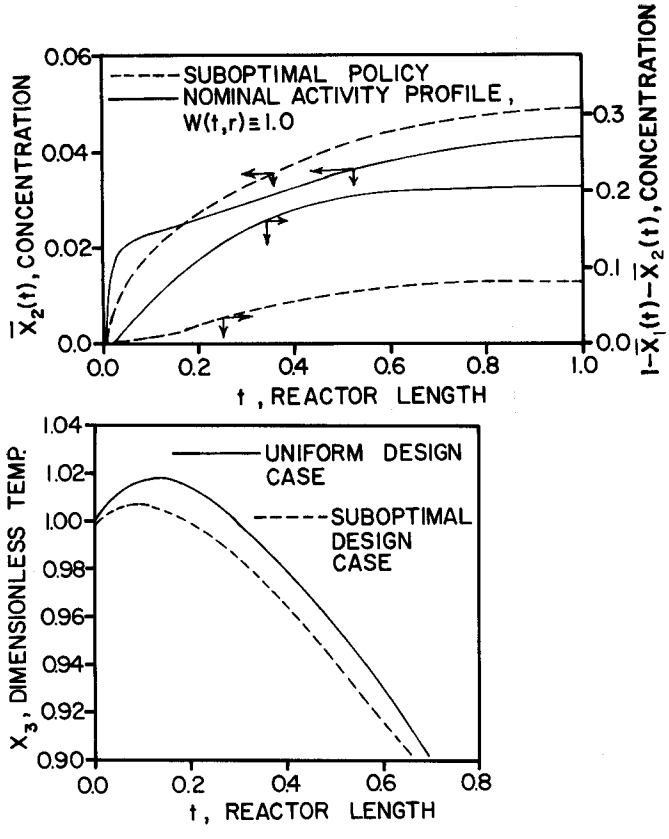

Fig. 9. Computed area-averaged product concentration (top) and reactor center temperature (bottom) for the reaction A→B→C with a pure bang-bang type of catalyst activity distribution.

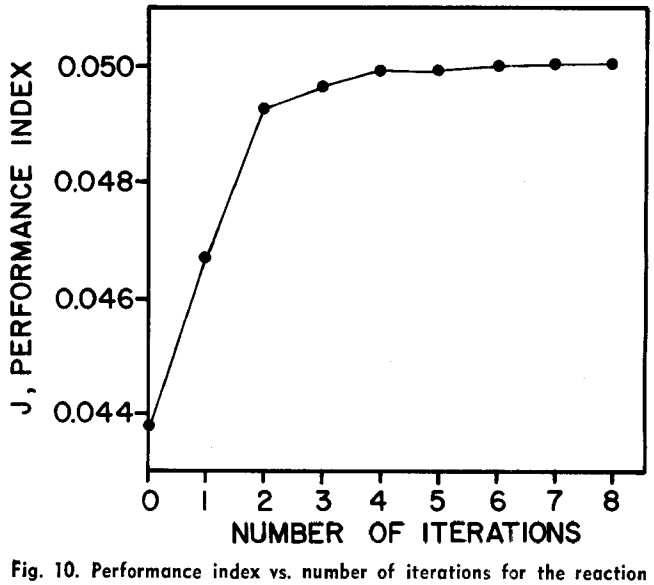

Fig. 10. Performance index vs. number of iterations for the reaction A→B→C with a pure bang-bang type of catalyst activity distribution.

plied to determine the pure bang-bang and the combined singular bang-bang types of catalyst activity distribution functions, $w(t, r)$. An implicit Crank-Nicholson finite difference scheme (Lapidus, 1962) was used to reduce (13) to (15) to a set of ordinary differential equations. In the finite difference discretization, 15 increments in the radial direction r and 100 increments in the axial direction t were employed. The nominal catalyst activity distribution function used throughout the following example calculations was assumed to be uniform, with $w(t, r) = 1.0$ for $0 \leq t \leq 1$ and $0 \leq r \leq 1$.

Computed results for the irreversible consecutive reaction $A \xrightarrow[k_1]{} B \xrightarrow[k_2]{} C$ with a pure bang-bang type of catalyst activity function used is shown in Figure 8. The computed suboptimal bang-bang type of catalyst distribution depicted in Figure 8 calls for $w(t, r) = 0.0$ along the center of the reactor entrance so as to reduce the hot spot temperature rise. This is further illustrated in the lower part of Figure 9, where the dimensionless temperature at the center of the reactor $r = 0$ is drawn against the axial reactor length t. It is seen that the highest reactor center temperature in the suboptimal bang-bang case is much lower than the corresponding temperature in the case of uniform catalyst activity distribution $w(t, r) = 0$ for $0 \leq t \leq 1$. In the upper part of Figure 9, the variation of the mean dimensionless concentrations of the desired product B and the undesired product C along the axial reactor length, namely, $\bar{x}_2(t)$ and $1 - \bar{x}_1(t) - \bar{x}_2(t)$, respectively, is shown. The results suggest that the bang-bang type of catalyst activity distribution function is not truly optimal and gives a value of performance index $\bar{x}_2(1) = 0.05010$, which is about 14% larger than that obtained by applying the initial uniform catalyst activity distribution $w(t, r) = 1.0$ for $0 \leq t \leq 1$ and $0 \leq r \leq 1$, that is, $\bar{x}_2(1) = 0.04383$. However, the latter uniform design produces considerably more undesired product C along the reactor than that obtained by using the suboptimal bang-bang catalyst activity distribution. Note that the stable and rapid convergence characteristics of the present algorithm demonstrated in the preceding lumped parameter system examples have also been observed in solving the nonlinear distributed parameter problems. This is illustrated in Figure 10, where the performance index $\bar{x}_2(1)$ is plotted against the number of iterations for the

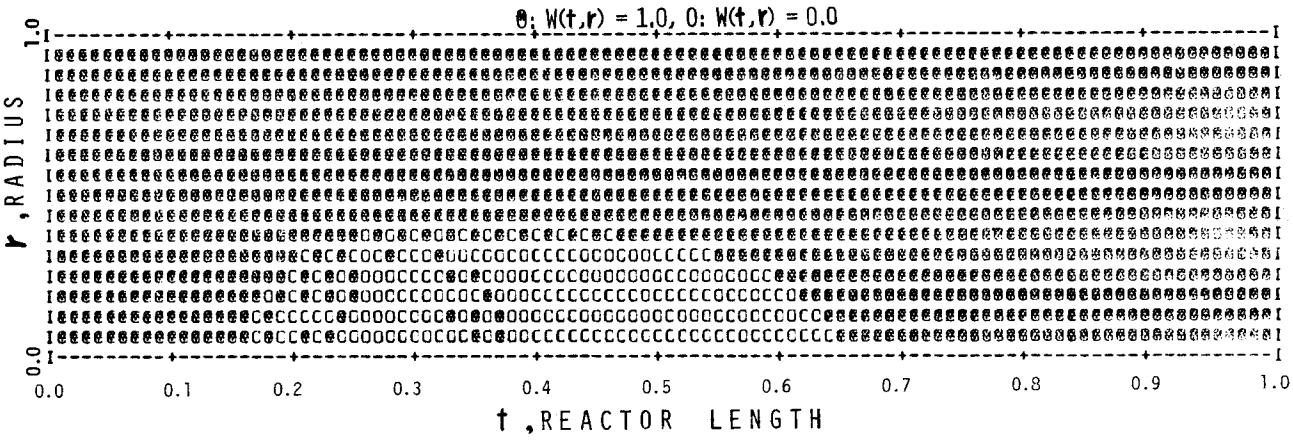

Fig. 11. Computed pure bang-bang type of catalyst activity distribution for the reaction A⇄B→C.

suboptimal bang-bang case. A total of eight iterations with a CPU time of 72 s on an IBM 370/155 computer was able to obtain the suboptimal bang-bang result. This corresponds to only 9 s of computation time per iteration. The computational efficiency of the present algorithm in solving the nonlinear distributed parameter problems is thus demonstrated quite favorably.

Figure 11 shows the computed suboptimal bang-bang type of catalyst activity distribution function $w(t, r)$ for the reversible consecutive reaction $A \underset{k_2}{\overset{k_1 \quad k_3}{\rightleftarrows}} B \rightarrow C$. The mean dimensionless concentration of the desired product B at the reactor effluent is $\bar{x}_2(1) = 0.46794$. Here, the nominal catalyst activity distribution function used in the iterative calculation is also a uniform one, namely, $w(t, r) = 1.0$ for $0 \leq t \leq 1$ and $0 \leq r \leq 1$, and this uniform design gives a value of $\bar{x}_2(1) = 0.45108$. By including an augmented quadratic performance index $\epsilon \int_0^{t_f} \mathbf{u}^T\mathbf{u}\, dt$ with a very small value of the variable weighting coefficient, say $\epsilon = 10^{-5}$, the computed singular bang-bang type of catalyst activity distribution function is depicted in Figure 12. The value of performance index is $\bar{x}_2(1) = 0.47475$, which is larger by only 1.45% than the corresponding value (0.46794) of the case with a pure bang-bang catalyst activity distribution. It then appears that the more easily implementable pure bang-bang type of catalyst activity distribution should be used for most practical purposes when compared with the singular bang-bang one.

It may be mentioned that the computational aspects of singular bang-bang control of nonlinear distributed parameter systems have received little attention. In particular, very few available computational algorithms have been demonstrated to be effective in solving the singular and/or bang-bang control problems in both nonlinear lumped and distributed parameter systems. In the literature, a combined approach in which the result from the direct search on performance index is used as the starting guess for the method of steep ascent has been shown by Seinfeld and Lapidus (1968*b*) to be quite feasible as a computational tool for handling some of these problems with particular chemical engineering interest. Thus, it seems worthwhile to comment briefly on the comparisons of the present algorithm with the approach of Seinfeld and Lapidus. First, in applying the approach of direct search on performance index to solve a pure lumped bang-bang control problem, the time interval $[0, t_f]$ is subdivided into a large number of segments. Within each segment, the control variables $\mathbf{u}(t)$ are chosen initially at their upper or lower bounds and then varied iteratively so as to improve the value of the specified performance index. If this approach is extended to solve problems involving the distributed control variables, $\mathbf{v}(t, r)$, however, the subdivision of the independent variables t and r has to be done in both coordinates. This will generally require an excessive amount of computer storage and computation time. For example, if the time interval $t \epsilon [0, t_f]$ is divided into L segments and the spatial coordinate $r \epsilon [0, 1]$ is discretized into N subintervals, then the distributed control variable $v(t, r)$ in a scalar, pure bang-bang control problem will have a total of $(L - 1) \times (N - 1)$ mesh point values. Thus, the system equation describing this distributed parameter system must be integrated $(L - 1) \times (N - 1)$ times in each overall itera-

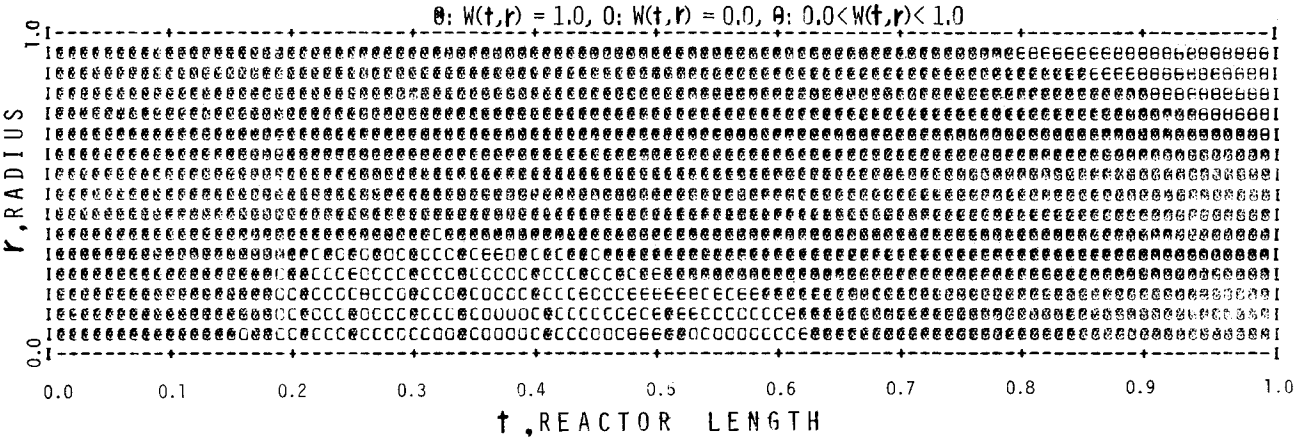

Fig. 12. Computed singular bang-bang type of catalyst activity distribution for the reaction A⇄B→C.

tive calculation. Even when a very coarse set of mesh points, say, $L = 11$ and $N = 11$, is used, the system equation must be integrated 100 times per iteration. Furthermore, if a singular control solution exists, a much finer set of time and spatial discretizations is normally required, and the number of integrations to be carried out will be increased at least several times. For the singular bang-bang control problems with multiple distributed control variables, the large number of iterations required should present some computational difficulties. Consequently, this seems to limit all the distributed singular bang-bang examples treated in Seinfeld and Lapidus (1968*b*) to problems with a scalar, boundary control variable only. In contrast, the present algorithm requires integrating the system and adjoint equations only once per iteration and requires the storage of the computed state variables only. Next, both the direct search procedure and the method of steep ascent used in the work of Seinfeld and Lapidus (1968*b*) are sensitive to the initial estimates of control variables; thus, several starting guesses of control variables are normally required when a problem is solved. This undesirable effect of the initial control guesses is also inherently existing in most gradient methods as well as in the preceding procedure of direct search of feedback gain matrix of Luus (1974*a*, 1974*b*) developed for lumped parameter minimum time control problems. The computational experience in using the present algorithm to solve all the lumped and distributed singular and/or bang-bang control system examples, however, has shown that the applicability of the algorithm is essentially independent of the initial control estimates regardless of the types of problems.

ACKNOWLEDGMENT

The financial supports provided by the National Science Foundation grant ENG 75-11293 and the Research Grant-in-Aid Program of Auburn University to Y. A. Liu, and the National Science Foundation grant GK-42622 to Leon Lapidus are gratefully acknowledged. Special appreciation is also extended to Mr. Kenji Nishihara for his assistance in part of this work.

NOTATION

$\mathbf{A}$ = system matrix
A = chemical component
$\mathbf{B}$ = control matrix
B = chemical component
C = chemical component
E_1, E_2 = activation energies
f = state equation
$\mathbf{H}$ = Hamiltonian function
$\mathbf{I}$ = identity matrix
J = performance index
J_c = augmented performance index
k_1, k_2, k_3 = reaction rate constants
$\mathbf{Q}$ = matrix of weighting coefficient
Q = dimensionless heat flux
r = spatial variable
R_1, R_2 = reaction rate expressions
t = time
t_f = final time
t_s = switching time
Δt = integration grid
$\mathbf{u}$ = control vector
w = catalyst activity distribution function
$\mathbf{x}$ = state vector
$\mathbf{x}_0$ = initial value of state vector
α = adiabatic temperature rise of the reaction
γ = ratio of the thermal capacities
ϵ = variable coefficient in the augmented performance index $\int_0^{t_f} \mathbf{u}^T\mathbf{u}\, dt$

Superscript

T = transpose of a vector or matrix

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Manuscript received November 26, 1975, and accepted January 29, 1976.

Trajectory Analysis of Deep-Bed Filtration with the Sphere-in-cell Porous Media Model

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This paper presents a model for the initial particle deposition in a deep-bed filter with a sphere-in-cell porous media model used. The analysis includes all the relevant mechanisms, and the results indicate that deposition occurs under favorable surface interactions. A semiempirical expression relating collection efficiency and operating parameters is presented.

SCOPE

The results reported in this study represent the continuing efforts of a long-range investigation whose objective is the development of a comprehensive theory of liquid filtration through granular beds. Such a theory of deep-bed filtration requires the selection of a mathematical and geometric model to characterize the bed for its hydrodynamic behavior and for its role as the collector of the particles in the suspension. The model chosen is then used to predict the dynamic behavior of the filtration process, that is, to predict the history of effluent quality and the corresponding change in the pressure drop across the filter. In this paper we employ the conceptually simple sphere-in-cell porous media model (Happel, 1958) to study the initial filtration efficiency with the help of the particle trajectory concept used in connection with other porous media models elsewhere (see Payatakes et al., 1974*a*, *b*, and *c*). The major objective of this work is to examine the use of this model for predicting initial collection rates in filters when the various filtration mechanisms such as sedimentation, interception, diffusion, and surface interactions act individually or collectively. Another important goal is to develop a semiempirical expression [Equation (27)] for the initial collection efficiency as a function of the pertinent process parameters. This is particularly desirable since such an expression would help avoid expensive computer work for future applications of this model.

CONCLUSIONS AND SIGNIFICANCE

The initial collection efficiency for filtration through granular beds is predicted within experimental error under a wide variety of conditions by the trajectory calculations made in this work with a sphere-in-cell porous media model. It is evident that an attractive surface force in the vicinity of the grains is required to permit filtration. Under such a condition, the collection rate depends on essentially four process parameters which characterize the ratio of the particle size to the grain size, the magnitude of the gravitational collection, the extent of the attractive