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An Effective Computational Algorithm for Suboptimal Singular and/or Bang-Bang Control

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I. Theoretical Developments and Applications to Linear Lumped Systems

A new and simple computational algorithm for obtaining suboptimal singular and/or bang-bang solutions of typical lumped and distributed parameter control problems is proposed. The algorithm is based on the piecewise maximization of the Hamiltonian and a limiting process utilizing a penalty function of the control variables. Theoretical developments and computational applications of the algorithm to several linear lumped parameter control problems are presented. Extensions and applications of the algorithm to nonlinear and distributed parameter systems are given in Part II.

SCOPE

The application of optimal control theory to dynamic systems of interest to the chemical process industry is often hampered by the existence of constraints, in addition to the common characteristics of these systems of having high state dimensionality, extreme nonlinearity, and multiple controls. The maximum principle formulation (Pontryagin et al., 1962) of such optimization problems leads to a nonlinear, two-point, boundary value problem which is difficult to solve numerically. Even though effective algorithms have been developed to calculate the optimal control policies for dynamic systems, the solution of many classes of optimization problems, especially those with nonlinear and distributed parameter characteristics, still requires excessive computation time and computer storage when these algorithms are applied. Suboptimal control is an attempt to approximate the solution to these problems with a reduced amount of computer storage and computation time. From a chemical engineering point of view, the use of suboptimal control is justified in many

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cases, because system models may not be very accurate, or because state measurements may not be precise. In addition, the use of suboptimal control may be justified for those problems where the performance index to be optimized is not sensitive to small perturbations in the control policy (Weber and Lapidus, 1971).

The present two-part paper is addressed to the development and application of a new, effective computational algorithm for obtaining the suboptimal solution of one of the most important and interesting problems which can arise in the theory of optimal control, namely, the singular and/or bang-bang control. Such a case may arise, for example, in a lumped parameter system when the Pontryagin Hamiltonian $H(x, \lambda, u)$, or simply H, is linear in the control variable(s) u. If the control variable is bounded, say, $u_* \leq u < u^* \leq \infty$, the optimal control, if it exists, is a bang-bang type and appears in the form

$$u(t) = \begin{cases} u^* & \phi(x, \lambda) > o \\ & o \leq t \leq t_f \\ u_* & \phi(x, \lambda) < o \end{cases}$$

where $\phi(x, \lambda)$, the so-called switching function, is the coefficient of u in the Hamiltonian, and u^* and u_* are the upper and lower bounds on the control variable u. However, when the Hamiltonian is not an explicit function of the control variable u over a finite time interval, the maximum principle fails to give adequate information for selecting the optimal control. When this occurs, the problem is referred to as a singular problem. The resulting optimal control may actually consist of a variable effort, with values intermediate between the upper and lower bounds of the control variable, which is called the optimal singular control.

Singular and/or bang-bang solutions have been known to appear in many optimal design and control problems of particular interest to chemical engineers. Siebenthal and Aris (1964) have shown the possible appearance of singular control in the optimal start-up of a continuous stirred-tank reactor. Other investigators, for example, Paynter and Bankoff (1966), Ko and Stevens (1971), and Edgar and Lapidus (1972*b*), have illustrated the occurrence of singular solutions in a variety of chemical reactor optimization problems. In a tubular reactor, the determination of the optimal use of mixed catalysts (Gunn and Thomas, 1965; Thomas and Wood, 1967; Jackson, 1968) and the calculation of the optimal catalyst activity distribution (Nishida et al., 1972) have also been shown to lead to a singular control problem. Optimal bang-bang solutions, which can occur in conjunction with optimal singular solutions, have been illustrated in the start-up or minimum-time control of a large number of processing units such as gas absorbers, liquid-liquid extraction trains, distillation columns, nuclear reactors, etc. Typical publications in this area are those of Chant and Luus (1968), Edgar and Lapidus (1972*a*, 1972*b*), Lapidus and Luus (1967), Lesser and Lapidus (1966), Luus (1974*c*), Mayar et al. (1970), Schlossmacher (1973), and others.

Recent studies on the analytical and computational aspects of the singular and/or bang-bang control problem have been discussed by such authors as Bell (1975), Edgar and Lapidus (1972*a*, 1972*b*), Ko and Stevens (1971*a*, 1972*b*), Davison and Monro (1971), Jacobson and Speyer (1971), and Seinfeld and Lapidus (1968*b*). While considerable progress has been made in the definition and characterization of the appearance of singular and/or bang-bang control, and in the derivation of necessary and sufficient conditions for optimal singular and/or bang-bang control, the control synthesis problem is still largely unsolved. In particular, very few computational algorithms have been demonstrated to be effective in solving the singular and/or bang-bang control problems in both lumped and distributed parameter systems with high state dimensionality, extreme nonlinearity, and multiple controls. Without obtaining the actual computational solution of a given control problem, it is usually impossible to establish the existence of singular control. Thus, the development of an effective computational algorithm to solve the singular and/or bang-bang control problem presents a serious challenge.

In the present work, a new and simple computational algorithm for obtaining the suboptimal singular and/or bang-bang solutions of typical lumped and distributed parameter control problems is developed. The proposed algorithm is based on the piecewise maximization of the Hamiltonian (Piecewise Max-*H*). Included in the algorithm is also a limiting process utilizing a penalty function of the control variables suggested by Jacobson et al (1970) and demonstrated by Edgar and Lapidus (1972*a*, 1972*b*) which solves the singular and/or bang-bang problem as the limit of a series of nonsingular and/or nonbang-bang problems. A number of examples have been computed to illustrate the effectiveness of the algorithm for solving large dimensional linear lumped parameter control problems with multiple controls. The application of the algorithm to several nonlinear lumped and distributed parameter control problems of particular chemical engineering interest is described in Part II of this work.

CONCLUSIONS AND SIGNIFICANCE

The present work demonstrates a new and simple computational algorithm for solving the suboptimal singular and/or bang-bang control problem. Specifically, in this paper and in Part II, the proposed piecewise maximization of the Hamiltonian and penalty function algorithm has been applied successfully to many typical lumped and distributed parameter systems with high state dimensionality, extreme nonlinearity, and multiple controls of particular chemical engineering interest. Based on the theoretical developments and computational examples presented in this work, the following advantages and disadvantages of the algorithm can be summarized.

1. The algorithm has been shown to be very effective in solving large dimensional optimal control problems with multiple controls. For example, the minimum time control problem of a twenty-state and seven-control linear lumped parameter system representing the linearized dynamic behavior of many stagewise processes in chemical engineering has been solved. This system seems to be one of the highest-order minimum time control problems that have ever been reported.

2. The algorithm permits large changes in the control in the iterative control calculations. In addition to having an assured convergence of the iterative control calculations, the algorithm also has very rapid convergence characteristics. For all the examples considered, nearly optimal singular and/or bang-bang control solutions have been successfully obtained within five to ten iterations, regardless of the values of the initial control estimates.

3. A general computer program for implementing the algorithm can be developed very easily, requiring only the routines for the state and adjoint equations and the

piecewise maximization of the Hamiltonian. The required computer memory is quite small, and the only stored variables are the state variables. All the computer calculation and storage of the auxiliary functions of the Hamiltonian such as H_u, H_{uu}, H_{ux}, $H_{u\lambda}$, etc., required in other control vector iteration methods are completely eliminated. The algorithm is also generally applicable to all types of performance indexes with both fixed and nonfixed final times.

4. When applied to any optimal control problem in which the Hamiltonian is a linear or a convex function of the control subject to the constraint $u_* \leq u \leq u^* < \infty$, the piecewise Max-$H$ algorithm will always give a nearly optimal pure bang-bang solution, even when the given optimal control problem may be a singular one. The disadvantage of this approach is that the exact optimal switching times of control variables are not calculated. The demonstrated advantages in applying the piecewise Max-H algorithm along with the penalty function approach to solve a large number of typical chemical engineering singular and/or bang-bang control problems in comparison with existing methods described in this paper and in Part II should suggest that the above limitation on the Hamiltonian for obtaining the pure bang-bang control is not a serious one.

THEORETICAL DEVELOPMENTS

In this paper, an effective computational algorithm for solving the singular and/or bang-bang control problem in both lumped and distributed parameter systems is developed. An explicit mathematical description of this singular and/or bang-bang control problem based on the maximum principle can be found in Seinfeld and Lapidus (1968*b*) and will not be repeated here. The recent papers by Ko and Stevens (1971*a*, 1971*b*) and Edgar and Lapidus (1972*a*, 1972*b*), as well as textbooks by Bryson and Ho (1969, pp. 246-270) and Kirk (1970, pp. 291-308), also contain useful information on the subject.

The method is based on the approach of approximation to the solution or approximation in the policy space (Lapidus and Luus, 1967; pp. 243-273). In the conventional approach to this approximate method based on the maximum principle, the system and the auxiliary adjoint equations as well as the associated boundary conditions are fixed. An iterative technique which involves a linearization procedure followed by a control correction scheme is developed to compute the control so as to achieve the convergence and maximization of the performance index. Most control correction schemes used in this approach *require* the computer calculation and storage of the auxiliary functions of the Hamiltonian such as H_u, H_{uu}, H_{ux}, $H_{u\lambda}$, etc. Also, every suboptimal state and control trajectories calculated by this approach will satisfy the system and adjoint equations along with their boundary conditions but will *not* maximize the Hamiltonian and the performance index. Typical iterative procedures included in this approach are the gradient and the second-variation methods, and their computational advantages and disadvantages in solving the singular and/or bang-bang control problem have been well-documented in the literature (Edgar and Lapidus, 1972*a*, 1972*b*; Ko and Stevens, 1971*a*, 1971*b*; Seinfeld and Lapidus, 1968*b*). For example, it is well-known that the use of a linear approximation in a gradient search procedure is an excellent means for arriving at the neighborhood of the desired value of optimal control quickly starting from almost any initial control policy. Near the optimum or over certain intervals in which the gradient of the Hamiltonian in the control space H_u is small in magnitude, the changes in the control $\mathbf{u}$ will be small so that the gradient procedure tends to exhibit poor convergence properties. On the other hand, the second-variation method, although cumbersome from a computational point of view, converges more quickly as the optimum point is approached. Thus, it has been suggested that the gradient and second-variation methods are best used together by first allowing the gradient method to reach close to the optimum trajectory and by switching to the second-variation method for refinement (Lapidus and Luus, 1967). This combined approach has been demonstrated to be feasible in solving the singular and/or bang-bang control problems (Ko and Stevens, 1971*a*, 1971*b*). Another method in the approach of approximation in the policy space which has been shown to permit large changes in the control $\mathbf{u}$ and to accelerate the convergence of the gradient method near the optimum is the Min-H strategy presented by Kopp and Moyer (1966), Gottlieb (1967), Gibson and Lowingen (1974), and others. In the terminology of the present work of referring to the maximum principle, instead of the minimum principle, an equivalent term for this method is the Max-H strategy. Briefly, a Max-H strategy is one that seeks, along a nonoptimum trajectory, that value of the control $\mathbf{u}$ which drives the gradient of the Hamiltonian in the control space H_u to zero. In the Max-H strategy presented by Gottlieb (1967) and by others, the iterative control correction scheme utilizes both the gradient and the second variation of the Hamiltonian in the control space, namely, H_u and H_{uu}, but it does not use the other second-order partial derivative of the Hamiltonian such as H_{ux} and $H_{u\lambda}$ as required in the conventional second-variation method. Although the Max-H strategy has been shown to be effective in solving many classes of optimal control problems, slow convergence or even divergence characteristics has still been observed in some applications reported in the literature (Gibson and Lowinger, 1974). Thus, it has been suggested that the Max-H strategy is best used as a terminal refinement scheme near the optimum in conjunction with other gradient-based methods (Kopp and Moyer, 1966), or some interpolative schemes should be used with the Max-H strategy to improve the control vector iteration (Gibson and Lowinger, 1974). In addition, the applicability of the Max-H strategy in obtaining the optimal or suboptimal solutions of singular and/or bang-bang control problem has not been demonstrated in the literature.

Specifically, in this paper, a new and simple approach based on the *piecewise maximization of the Hamiltonian* (piecewise Max-H) is first proposed as an effective method for obtaining the suboptimal bang-bang solutions of typical lumped and distributed parameter optimal control problems. This new method will *always* give a bang-bang solution of a fairly high degree of suboptimality to any optimal control problem in which the Hamiltonian H is a linear or a convex function of the control $\mathbf{u}$ subject to the constraint $u_* \leq u \leq u^* < \infty$, even when the given optimal control problem may be a singular one. As will be illustrated in the subsequent sections and in Part II, this class of problems encompasses a very large number of typical optimal control problems of chemical engineering interest. An advantage of the proposed method is that it permits large changes in the control $\mathbf{u}$ in the iterative control correction scheme with assured rapid and uniform convergence

characteristics starting from any initial control policy. Another advantage of the new method is that all the computer calculation and storage of the auxiliary functions of the Hamiltonian such as H_u, H_{uu}, H_{ux}, $H_{u\lambda}$ required in the gradient, the second-variation, the Max-H, and other related methods in the approach of approximation in the control space are completely eliminated. *The proposed algorithm is generally applicable to optimal control problems with all types of performance indexes* (Hiratsuka, Nishida, Liu, and Lapidus, 1976). For convenience, the specific performance index chosen for the present singular and/or bang-bang control study is a scalar, quadratically weighted function of the values of state variables at the fixed or nonfixed final time t_f; namely, $J = \mathbf{x}^T(t_f)\mathbf{Q}\,\mathbf{x}(t_f)$, where $\mathbf{Q}$ is a proper weighting matrix.

For the typical linear or nonlinear lumped parameter optimal control problem with a fixed final time t_f, in which the Hamiltonian is a linear or convex function of the control $\mathbf{u}$ subject to the constraint $\mathbf{u}_* \leq \mathbf{u} \leq \mathbf{u}^*$, the following computational steps based on the piecewise maximization of the Hamiltonian can be used to find a suboptimal bang-bang control policy with $\mathbf{u} = \mathbf{u}_*$ or $\mathbf{u} = \mathbf{u}^*$.

1. Divide the time interval $(0, t_f)$ into N equidistant subintervals with $N\Delta t = t_f$, where Δt is the integration step size.

2. Assume an initial control policy $\mathbf{u}^o(t)$ for $0 \leq t \leq t_f$ and set the iteration number $m = 1$. The initial control policy can be expressed more specifically as a set of piecewise constant controls $\{\mathbf{u}^{m-1}(t)\colon \mathbf{u}^{m-1}(t) = \mathbf{u}^{m-1}(P\Delta t),\ (P-1)\,\Delta t < t \leq P\Delta t,\ P = 1, 2, \ldots, N\}$, $m = 1$, where $\mathbf{u}^{m-1}(P\Delta t)$ may be equal to $\mathbf{u}^{m-1}[(P-1)\Delta t]$.

3. Introduce an $(n+1)$-dimensional augmented state vector $\bar{\mathbf{x}}$ defined by $\bar{\mathbf{x}} = [\mathbf{x}\ x_{n+1}]^T$, where $\mathbf{x}$ is the original n-dimensional state vector satisfying the state equation $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u})$ with the initial condition $\mathbf{x}(0) = \mathbf{x}_o$, and x_{n+1} is an additional auxiliary state variable satisfying the equation $\dot{x}_{n+1} = \mathbf{x}^T\mathbf{Q}\,\mathbf{x}$ with the initial condition $x_{n+1}(0) = 0$. Integrate the augmented state equation $\dot{\bar{\mathbf{x}}}^m(t) = \mathbf{g}(\bar{\mathbf{x}}^m, \mathbf{u}^{m-1}) = [\mathbf{f}(\mathbf{x}^m, \mathbf{u}^{m-1})\ \mathbf{x}^{mT}\mathbf{Q}\,\mathbf{x}^m]^T$ forward from $t = 0$ to $t = t_f$ with the initial condition $\bar{\mathbf{x}}(0) = [\mathbf{x}(0)\ x_{n+1}(0)]^T = [\mathbf{x}_o\ 0]^T$ and store the computed values of the augmented state variables $\bar{\mathbf{x}}^m(t)$ and compute the performance index $J^{m-1}(\bar{\mathbf{x}}^m, \mathbf{u}^{m-1}) = \bar{\mathbf{x}}^{mT}(t_f)\,\mathbf{Q}\,\bar{\mathbf{x}}^m(t_f) = \bar{x}^m{}_{n+1}(t_f) = \bar{x}^m{}_{n+1}(N\Delta t)$.

4. Introduce the Hamiltonian $H(\bar{\mathbf{x}}, \boldsymbol{\lambda}, \mathbf{u}) = \boldsymbol{\lambda}^T\mathbf{f} + \lambda_{n+1}[\mathbf{f}^T\mathbf{Q}\,\bar{\mathbf{x}} + \bar{\mathbf{x}}^T\mathbf{Q}\,\mathbf{f}]$. Using the known values of the state and adjoint variables at $t = t_f = N\Delta t$, namely, $\bar{\mathbf{x}}^m(t_f)$ and $\boldsymbol{\lambda}^m(t_f) = -H_{\bar{\mathbf{x}}}(t_f) = \mathbf{c}$ (a known constant vector), carry out the maximization of the Hamiltonian $H(\bar{\mathbf{x}}^m, \boldsymbol{\lambda}^m, \mathbf{u})$ at $t = t_f = N\Delta t$ with respect to $\mathbf{u}$ to obtain a new control $\mathbf{u}^m(t) = \mathbf{u}^m(N\Delta t)$. Applying this resulting control as a piecewise constant control policy within the time subinterval $(N-1)\,\Delta t < t \leq N\Delta t = t_f$ and using the stored values of the state variables $\bar{\mathbf{x}}^m(t)$, integrate the adjoint equation $\dot{\boldsymbol{\lambda}}^m(t) = -H_{\bar{\mathbf{x}}}(\bar{\mathbf{x}}^m, \mathbf{u}^m, \boldsymbol{\lambda}^m)$ backward from $t = t_f = N\Delta t$ to $t = (N-1)\Delta t$ with the known boundary condition $\lambda^m(t_f) = -H_{\bar{\mathbf{x}}}(t_f) = \mathbf{c}$ (a known constant vector) to obtain $\boldsymbol{\lambda}^m\,(N-1)\Delta t$. Use the known values of the state and adjoint variables at $t = (N-1)\Delta t$, namely, $\bar{\mathbf{x}}^m\,[(N-1)\Delta t]$ and $\boldsymbol{\lambda}^m\,[(N-1)\Delta t]$, and apply the similar maximization procedure to find a new piecewise constant control, $u^m(t) = u^m\,[(N-1)\Delta t]$ for the time subinterval $(N-2)\Delta t < t \leq (N-1)\Delta t$. Repeat the same procedure until the complete set of the new piecewise constant controls $\{\mathbf{u}^m(t)\colon \mathbf{u}^m(t) = \mathbf{u}^m(P\Delta t),\ (P-1)\Delta t < t \leq P\Delta t,\ P = 1, 2, \ldots N\}$ is found, where $\mathbf{u}^m(P\Delta t)$ may be equal to $\mathbf{u}^m\,[(P-1)\Delta t]$.

5. Compute the performance index $J^m(\bar{\mathbf{x}}^m, \mathbf{u}^m)$ and compare with $J^{m-1}(\bar{\mathbf{x}}^m, \mathbf{u}^{m-1})$. If the difference between the subsequent performance indexes is within the preassigned tolerance, the iterative calculation is terminated and the desired control is $\mathbf{u}^m(t)$. Otherwise, return to step 2 by exchanging the previous control with the current control.

This piecewise Max-H algorithm is applicable to solve control problems with both fixed and nonfixed final time t_f. If the final time for a given control problem is not specified, the nonfixed final time problem can be solved as a series of fixed final time problems. This procedure will give many sets of meaningful and complete results for a single problem with the final time as a parameter. The iterative optimization of the unspecified final time terminates when the performance index converges to its maximum value. Also, since the time grid for the digital integration of the state and adjoint equations and the piecewise maximization of the Hamiltonian may not be the same as the optimal switching time for the control, the bang-bang control policy computed by this piecewise Max-H algorithm is suboptimal in most cases.

When a given optimal control problem may be singular, because the state equation is nonlinear or because the Hamiltonian is not an explicit function of the control $\mathbf{u}$ over a finite time interval, etc., a penalty-function limiting process suggested by Jacobson et al. (1970) and demonstrated by Edgar and Lapidus (1972*a*, 1972*b*) is proposed as an augmenting procedure in conjunction with the new approach of the piecewise maximization of the Hamiltonian for obtaining the suboptimal singular and bang-bang solutions of typical lumped and distributed parameter optimal control problems. This limiting process involves the augmenting of the original performance index $J = \bar{\mathbf{x}}^T(t_f)\mathbf{Q}\,\bar{\mathbf{x}}(t_f)$ with an integral quadratic control term $\int_o^{t_f} \mathbf{u}^T\mathbf{u}\,dt$ multiplied by a variable coefficient ϵ. In other words, the augmented performance index $J_c = \bar{\mathbf{x}}^T(t_f)\,\mathbf{Q}\,\bar{\mathbf{x}}(t_f) + \epsilon\int_o^{t_f} \mathbf{u}^T\mathbf{u}\,dt$ is used. With the addition of the integral quadratic control term, the control problem loses its singular and/or bang-bang characteristics. However, in the overall computational solution of a given control problem, the variable coefficient ϵ is sequentially reduced until it approaches zero, and the original singular and/or bang-bang control problem is solved in the limit. Hence, in the solution of a singular and/or bang-bang control problem, the present algorithm employs the penalty function limiting process to convert the problem to a series of nonsingular and/or nonbang-bang problems and then uses the piecewise maximization of the Hamiltonian to obtain the desired control policy in each successive iterative calculation. The specific computational procedures for incorporating this penalty function limiting process to the proposed piecewise Max-H algorithm are very simple and essentially similar to those presented by Edgar and Lapidus (1972*b*), who have combined the same limiting approach with a discrete dynamic programming procedure to solve the singular bang-bang control problems. The details will be omitted here.

It is worthwhile to mention that in the present work, the piecewise maximization of the Hamiltonian is carried out over the whole time interval of interest to the control problem, namely, $[0, t_f]$. A more general algorithm in which the piecewise Max-H algorithm is applied only to some time subintervals, say $\tau\epsilon[0, t_f]$, has also been developed (Hiratsuka, Nishida, Liu, and Lapidus, 1975). In particular, the following theorem and corollary which charac-

TABLE 1. THREE LINEAR LUMPED PARAMETER SYSTEMS

	System 1: second order two controls	System 2: fourth order one control	System 3: twentieth order seven controls
References	Tou (1964)	Plant and Athans (1966) Jacobson (1968	
System matrix A	$\begin{bmatrix} 0 & -1 \\ 2 & -3 \end{bmatrix}$	$\begin{bmatrix} -0.5 & 5 & 0 & 0 \\ -5 & -0.5 & 0 & 0 \\ 0 & 0 & -0.6 & 10 \\ 0 & 0 & -10 & 0.6 \end{bmatrix}$	A (20 × 20) tridiagonal matrix
Input matrix B	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}$	B (20 × 7) matrix with elements: $b_{ij} = \begin{cases} 1 & i = 3j \quad i = 1, 2, \ldots 20 \\ 0 & i \neq 3j \quad j = 1, 2, \ldots 7 \end{cases}$
Initial condition $\mathbf{x}(0) = \mathbf{x}_0$	$x_i(0) = 1; i = 1, 2$	$x_i(0) = 10; \quad i = 1, 2, 3, 4$	$x_i(0) = 1; \quad i = 1, 2, \ldots 20$

terize the convergence properties of the more general and the present specific algorithms can be stated when the time grid of integration is very small.

Theorem

There always exists a time subinterval $\tau^m \epsilon [0, t_f]$ such that $J^m(\bar{\mathbf{x}}^m, \mathbf{u}^m) < J^{m-1}(\bar{\mathbf{x}}^m, \mathbf{u}^{m-1})$ when the piecewise Max-H algorithm is applied over the time subinterval τ^m to modify the control variables.

Corollary

Suppose the Hamiltonian is a linear or a convex function of the state variables. The uniform convergence of the iterative control calculations is guaranteed if the piecewise Max-H algorithm is applied over the whole time interval, that is, when $\tau^m = [0, t_f]$.

The proofs of these results will be reported separately (Hiratsuka, Nishida, Liu, and Lapidus, 1976). In the present work, it is sufficient to check the validity of the assured convergence characteristics of the iterative control calculations stated by the corollary through the computational results of the system examples.

SYSTEM EXAMPLES

Three Standard Linear Lumped Parameter Systems

The first three linear lumped parameter systems investigated were modeled by the standard system equation of the form

$$\dot{\mathbf{x}}(t) = \mathbf{A}\,\mathbf{x}(t) + \mathbf{B}\,\mathbf{u}(t) \tag{1}$$

$$\mathbf{x}(0) = \mathbf{x}_0 \tag{2}$$

and their details are shown in Table 1. It is desired to find the optimal control $\mathbf{u}(t)$ satisfying (1) and (2) and the constraint

$$-1 \leq u_k \leq 1 \qquad k = 1, 2, \ldots, r \tag{3}$$

which will drive the state vector $\mathbf{x}(t)$ from its initial state $\mathbf{x}(0)$ to the origin in minimum time. As shown in Table 1 and Equations (1) and (2), since the control variables in all the first three systems are bounded and appear linearly in the system equation, the maximum principle by Pontryagin will suggest that an optimal control is of the bang-bang type. System 1 was solved by Tou (1964) using a state-transition formulation, system 2 by Plant and Athans (1966) using a boundary condition iteration method, as well as by Jacobson (1968) using a differential dynamic programming approach. The twenty-state, seven-control linear system, system 3, has not been examined in the previous studies. This system seems to be one of the highest-order time optimal control problems that have ever been reported. The tridiagonal form of the system matrix A in system 3 is often encountered in the linearized dynamic modeling of many stagewise processes in chemical engineering.

Optimal Use of Mixed Catalysts for Two Successive Reactions in a Tubular Reactor

The final linear lumped parameter system is of more direct chemical engineering interest. The problem of determining the optimal catalyst blending policy as a function of the axial position along a tubular reactor in which a bifunctional catalytic, consecutive reaction occurs under isothermal conditions was investigated. Consider the following consecutive reaction scheme (Gunn and Thomas, 1965; Thomas and Wood, 1967; Jackson, 1968)

$$A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B \xrightarrow{k_3} C \tag{4}$$

and denote the mole fractions of the substances A and B by x_1 and x_2, respectively. The differential equations describing the variation of composition with the axial distance along the reactor are

$$\dot{x}_1(t) = u\,(k_2 x_2 - k_1 x_1) \tag{5}$$

$$\dot{x}_2(t) = u\,(k_1 x_1 - k_2 x_2) - (1 - u)\,k_3 x_2 \tag{6}$$

where t represents the residence time of the substances from the instant of entry to the reactor. The symbols k_1 and k_2 are, respectively, the reaction rate constants of the first two reactions in a reactor where the catalyst consists entirely of the substance which catalyzes the reversible reactions $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$, while the symbol k_3 is the reaction rate constant of the third reaction in a reactor where the catalyst consists entirely of the substance which catalyzes the reaction $B \xrightarrow{k_3} C$. The catalyst blending fraction u is the fraction of the catalyst formed by the substance which catalyzes the reaction $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$; this fraction can be varied along the axial position of the reactor. Obviously, the physical constraint on the catalyst blending fraction requires

$$0 \leq u(t) \leq 1 \tag{7}$$

The problem is to find the optimal catalyst blending policy $u(t)$ subject to the constraint (7) so as to maximize the reactor performance index J, namely, the mole fraction of

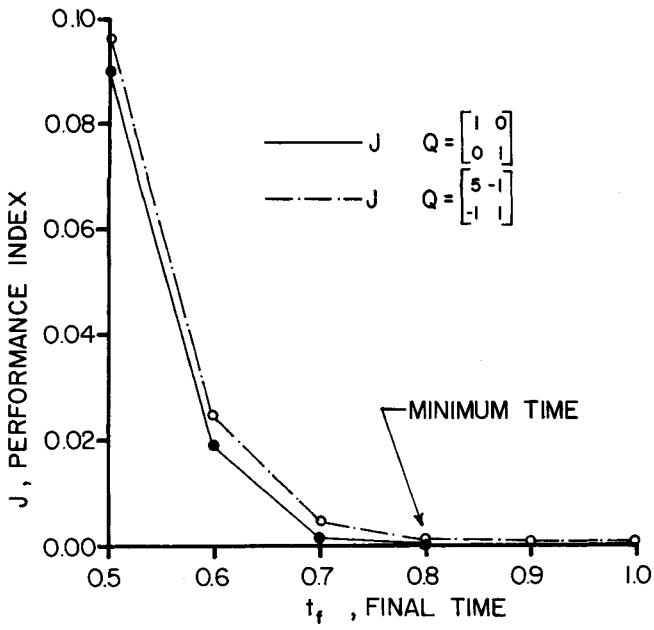

Fig. 1. Performance index vs. final time for system 1 with two different weighting matrices: suboptimal bang-bang control.

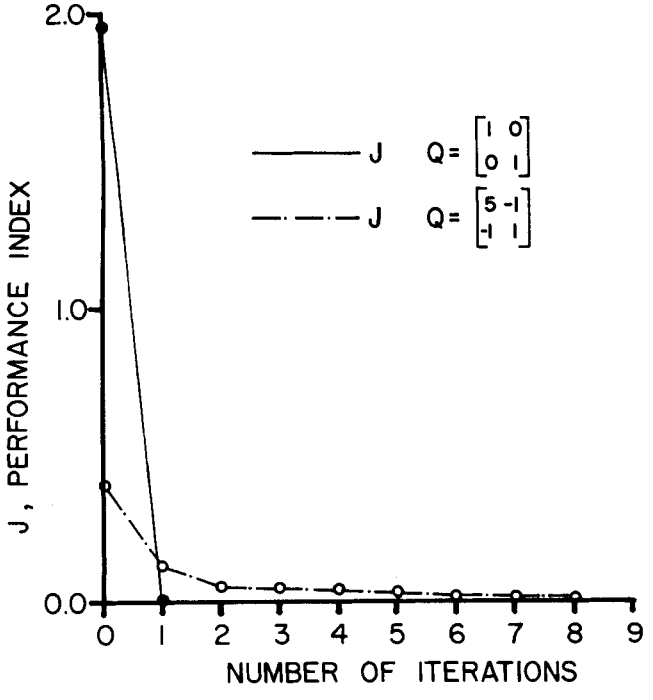

Fig. 2. Performance index vs. number of iterations for system 1 with final time $t_f = 0.8$ and two different weighting matrices: suboptimal bang-bang control.

the substance C present in the mixture at the reactor exit $t = 1$:

$$J = 1 - x_1(1) - x_2(1) \tag{8}$$

The control variable $u(t)$ is bounded and appears linearly in the system Equations (5) and (6). The maximum principle by Pontryagin seems to indicate an optimal control of the bang-bang type. However, the nonseparable form of the state and control variables in (5) and (6) suggests that a singular arc will occur in which the catalyst blending fraction $u(t)$ varies with value intermediate from 1 to 0 along certain axial positions of the reactor. Indeed, there are some quite sound physical and economical justifications for the appearance of such a singular arc in using mixed catalysts in a single reactor rather than carrying out the two successive reaction steps in two reactors separately. The details can be found in Thomas and Wood (1967) and in Jackson (1968). In the former article, a suboptimal solution to this problem by using a gradient method was also given. A complete, analytical, optimal solution in closed form to the problem, however, was presented by Jackson (1968) using the maximum principle.

NUMERICAL RESULTS

In this section, numerical results obtained on the suboptimal singular and/or bang-bang control of the preceding system examples with the proposed computational algorithm are presented. The important considerations in illustrating the feasibility and efficiency of the present suboptimal procedure as the convergence characteristics, the degree of suboptimality, the effect of initial control estimate, the choice of performance index, the effect of integration grid, etc., are discussed. Both fixed and nonfixed final time problems are included, and the results are also compared with other published studies.

Minimum Time Control of Three, Standard Linear Lumped Parameter Systems

The minimum time control for the first three linear lumped parameter systems represented by Equations (1) and (2) has been solved by choosing the control policy for each system to reach the origin ($\mathbf{x} = \mathbf{0}$) from the given initial condition [$\mathbf{x}(0) = \mathbf{x}_0$] specified in Table 1 for different value of final time t_f according to the computational algorithm described in the preceding section. Figure 1 shows the change in the performance index $J = \mathbf{x}^T(t_f)\,\mathbf{Q}\,\mathbf{x}(t_f)$ of system 1 for a series of final times and two different weighting matrices:

$$\text{case 1: } \mathbf{Q} = \mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{case 2: } \mathbf{Q} = \begin{bmatrix} 5 & -1 \\ -1 & 1 \end{bmatrix}$$

Since no substantial improvement index can be observed after $t_f = 0.8$, the minimum time required for system 1 to reach the origin is taken as 0.8. To indicate the rapid convergence characteristics in applying the present algorithm, the performance index is plotted against the number of iterations in Figure 2 for system 1 with $t_f = 0.8$ and both weighting matrices. In both cases, the performance indexes decrease to zero rapidly with a very few number of iterations. In particular, for the case with $\mathbf{Q} = \mathbf{I}$, the performance index decreases to an almost zero value with only one iteration. As will be shown in the other numerical results to be described, such a rapid convergence characteristic is typical in applying the present algorithm to all the system examples considered with a fixed or nonfixed final time. The computation time required for obtaining these results is quite small. For example, for case 2 with an nonidentity weighting matrix, a CPU time of 5 s on a FACOM 230/60 computer is needed when an integration step of $\Delta t = 0.02$ is used between $t = 0$ and $t = t_f = 0.8$. Figure 3 depicts the computed control policy for system 1 with $t_f = 0.8$ and the above two weighting matrices. It is seen that the choice of weighting matrices affects the number of control switches. Also, Figures 1 to 3 illustrate that for both fixed and nonfixed final time problems, it is possible to improve the problem solution by properly choosing the weighting matrix $\mathbf{Q}$ in the quadratic performance index $J = \mathbf{x}(t_f)^T\,\mathbf{Q}\,\mathbf{x}(t_f)$. Although no attempt has been made in optimally choosing the weighting matrix in the present work, a number of methods for such a purpose were given by Lapidus and Luus (1967), Chant and Luus (1968), Bennett and Luus (1971), Schlossmacher and Lapidus (1971), Luus and Jaakola (1973), Luus (1974*c*), and others.

The effect of integration step size in applying the present computational algorithm may be illustrated with

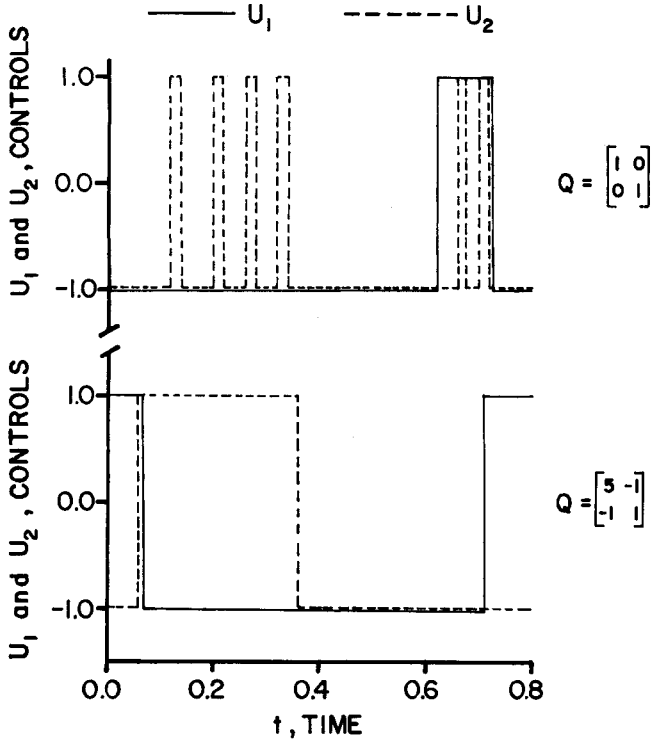

Fig. 3. Computed suboptimal bang-bang control trajectories for system 1 with final time $t_f = 0.8$ and two different weighting matrices.

the results of the suboptimal bang-bang control of system 2. Here, a fixed final time problem with $t_f = 4.2$ (Plant and Athans, 1966; Jacobson, 1968) may be considered. It is desired to find the proper integration step size so that the performance index $J = \mathbf{x}^T(4.2)\mathbf{x}(4.2)$ is smaller than 1.0. The computed values of performance index for several integration stepsizes are shown below:

Integration step size, Δt	0.0084	0.004	0.002	0.0005
Performance index, J	1.2688	1.1279	1.0551	0.9952

These suggest that an integration grid of $\Delta t = 0.0005$ provides a valid solution to the problem. The resulting value of performance index $J = 0.9952$ is slightly smaller than the value of 0.9960 obtained by Jacobson (1968) using a differential dynamic programming approach. The computed suboptimal bang-bang control policy begins with an initial control $u = -1.0$ at $t = 0.0$ and switches between the control constraints $u = -1.0$ and $u = 1.0$ until $t_f = 4.2$ at the following switching times: $t_s = 0.1405$, 0.9205, 1.3745, 2.1700, 2.6210, 3.4345, and 3.8740. These switching times are approximately the same as those given by Jacobson; however, the exact switching times are not calculated by the present algorithm.

System 3 with twenty-state and seven-control provides an ultimate test of the proposed algorithm in solving typical chemical engineering problems with high state dimensionality and multiple controls. The computed values of performance index $J = \mathbf{x}^T(t_f)\ \mathbf{x}(t_f)$ with several values of final time t_f are as follows:

Final time, t_f					
1.02	1.04	1.06	1.10	1.20	1.30
Performance Index $J = \mathbf{x}^T(t_f)\ \mathbf{x}(t_f)$					
0.01796	0.01633	0.01250	0.00716	0.00695	0.0083

Thus, a minimum time of $t_f = 1.10$ with the performance index $J < 0.01$ may be chosen .This computation requires 27 s of CPU time on a FACOM 230/60 computer with an

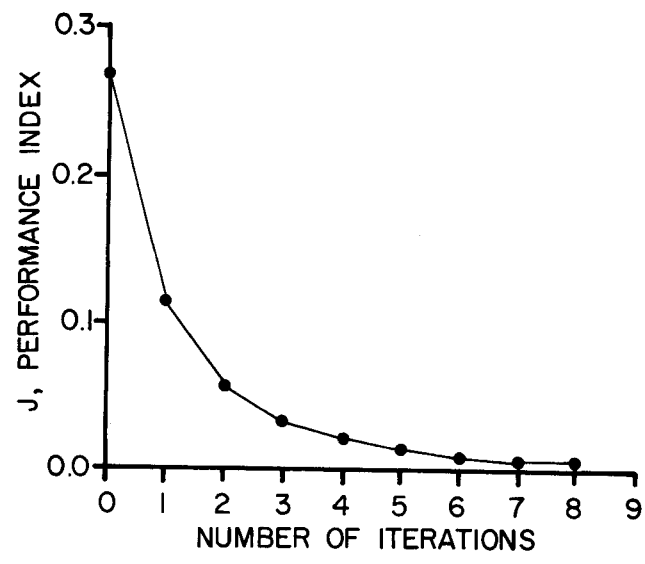

Fig. 4. Performance index vs. number of iteration for system 3 with final time $t_f = 1.10$: suboptimal bang-bang control.

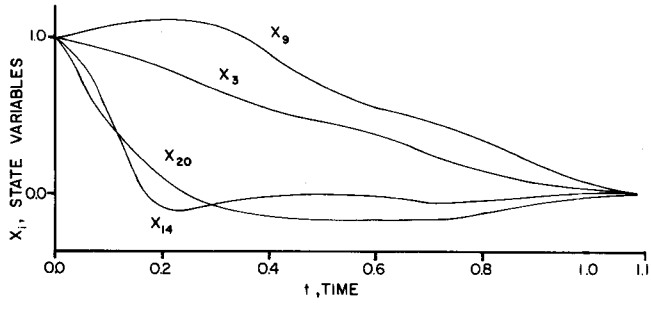

Fig. 5. Computed state trajectories for system 3 with final time $t_f = 1.10$: suboptimal bang-bang control.

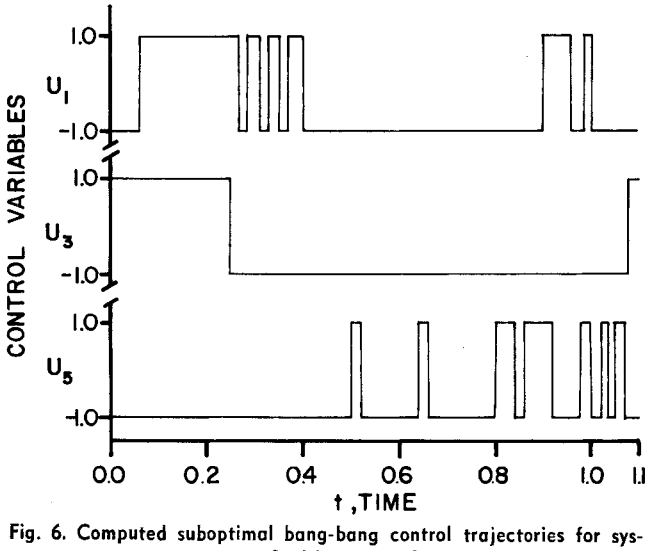

Fig. 6. Computed suboptimal bang-bang control trajectories for system 3 with $t_f = 1.10$.

integration step of $\Delta t = 0.02$ between $t = 0$ and $t = t_f = 1.10$. Figure 4 shows the change in the value of performance index with the number of iterations for $t_f = 1.10$. It is evident that the convergence characteristic in applying the proposed method to this higher-order system is again quite rapid, with the reduction from $J = 0.2548$ to $J = 0.00716$ achieved only in eight iterations. The typical trajectories of state variables x_3, x_9, x_{14}, and x_{20} and the corresponding suboptimal bang-bang controls u_1, u_3, and u_5 are illustrated in Figures 5 and 6. It should be mentioned that in applying the proposed algorithm to solve this higher-order system and other system examples

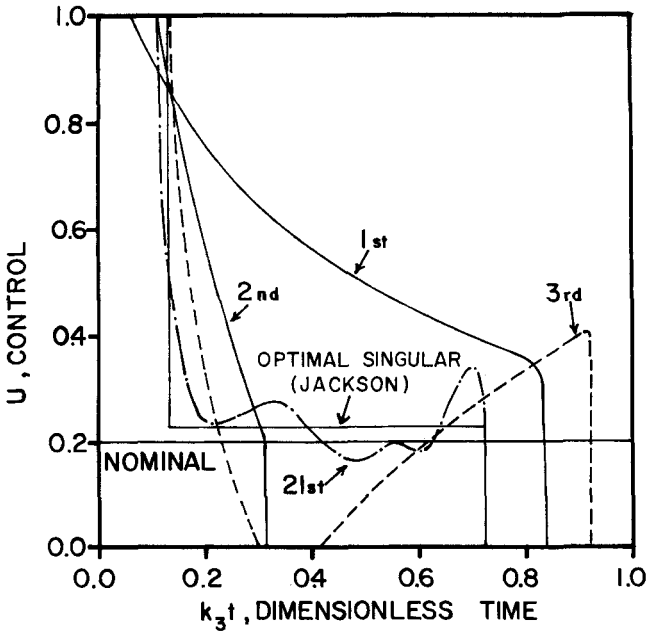

Fig. 7. Computed catalyst blending fraction u vs. dimensionless time (reactor length) in successive number of iterations for the catalyst blending problem: singular bang-bang control.

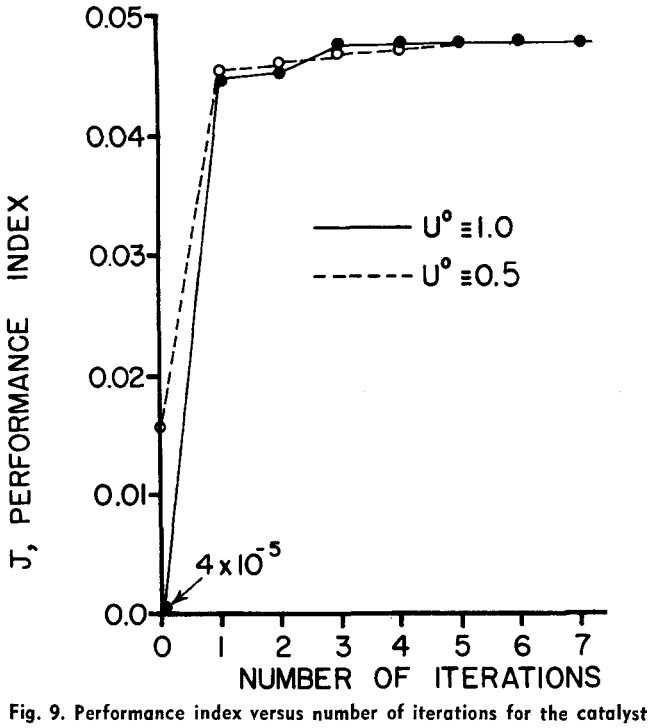

Fig. 9. Performance index versus number of iterations for the catalyst blending problem: pure bang-bang control.

considered in this work, it is not necessary to have any prior information on the final optimal or suboptimal control. Any allowable choice of the initial control estimate such as the lower or the upper bound of each control variable has been found to be successful in obtaining the problem solution without affecting the convergence characteristic, the degree of suboptimality, etc. This fact is further illustrated in the following example.

Optimal Use of Mixed Catalysts for Two Successive Reactions in a Tubular Reactor

The combined singular bang-bang control algorithm developed in the preceding section has been applied to determine the best catalyst blending fraction as a function of the axial position along a tubular reactor so as to maxi-

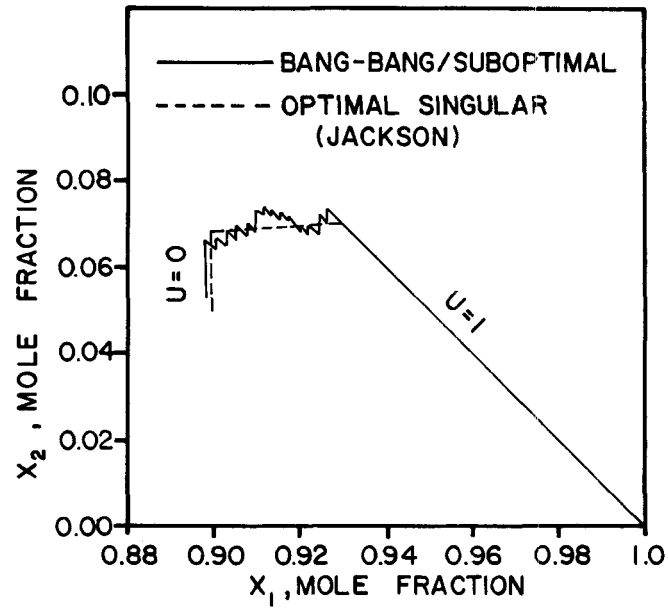

Fig. 8. Computed phase plane for the catalyst blending problem: pure bang-bang control and singular bang-bang control by Jackson (1968).

mize the mole fraction of the product C at the reactor exit for the isothermal bifunctional, catalytic, consecutive reaction $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B \xrightarrow{k_3} C$. By using the same values of reaction rate constants and final time as in the studies by Gunn and Thomas (1965) and by Jackson (1968), namely, $k_1 = k_3 = 1.0$, $k_2 = 10.0$ and $t_f = 1.0$, the computed catalyst blending fraction $u(t)$ is shown as a function of the dimensionless reactor holding time k_3t in Figure 7. The computed catalyst blending policy shown in Figure 7 is almost identical with the optimal one calculated analytically by Jackson (1968), especially when the variable coefficient ϵ in the augmented performance index $\epsilon \int_0^{t_f} \mathbf{u}^T \mathbf{u}\, dt$ approaches zero. It can also be seen from Figure 7 that the computed control trajectories in successive iterations are quite far from each other. This is a typical example illustrating the capability of the proposed algorithm in obtaining large changes in the values of control variables. In other words, the present algorithm can always provide a global variation in the control variables so as to speed up the convergence of the iterative calculation. This compares favorably with many other gradient and second variation methods, which can only iteratively vary the values of control variables locally and normally require a fairly large number of iterations before achieving convergence. The computation time for the proposed algorithm to solve this singular bang-bang problem is 15 s of CPU time on IBM 370/155 computer with 250 integration steps, each iteration requiring less than 0.6 s.

Next, a pure bang-bang catalyst blending policy was also calculated by the algorithm. This is equivalent to determining the best use of a pure catalyst which catalyzes either the reaction $A \underset{k_2}{\overset{k_1}{\rightleftarrows}} B$ or the reaction $B \xrightarrow{k_3} C$ only. The computed results are shown in a phase plane of the state variables x_1 and x_2 in Figure 8, where the optimal singular catalyst blending policy calculated analytically by Jackson (1968) is also included. The policy of using a pure catalyst which catalyzes the reaction $B \rightarrow C$ only, namely, $u = 0$, corresponds to a segment parallel to the x_2 axis, while the segment marked as $u = 1$ in Figure 8 corresponds to using

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.

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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-