The Computation of Optimal Singular Bang-Bang Control II. Nonlinear Systems

A general algorithm for the computation of singular/bang-bang control, previously applied to linear systems, is extended to nonlinear systems. The minimum time control of a two-stage CSTR is demonstrated.

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SCOPE

In the preceding paper by Edgar and Lapidus (1972) it is shown how optimal singular/bang-bang control can be computed for linear systems with fixed or nonfixed final times. The computation utilizes the conversion of the given control problem into a linear-quadratic problem (LQP), which is then solved via discrete dynamic programming with discrete penalty functions to handle end point and control constraints. Inherent in the problem solution is a limiting process, which solves the singular/bang-bang problem as the limit of a series of nonsingular/non-bang-bang problems.

In this work it will be shown how a singular/bang-bang control problem with a nonlinear system equation can be converted into an LQP. The method of solution for the LQP is the same as that mentioned earlier; however, the calculated control is suboptimal, as opposed to the optimal control which results for linear systems. The calculated control is suboptimal because the nonlinear state equations are approximated as time-varying linear state equations. The suboptimal control estimate is then refined by first-order and second-order descent methods in conjunction with the limiting process to yield the optimal singular/bang-bang control.

A number of nonlinear system reactor engineering examples have been computed to test the effectiveness of the proposed algorithm. The optimal startup control of a four-state variable system, a problem which cannot be solved by the method of phase plane analysis, has been computed by the new algorithm and is presented here. The results demonstrate that the new algorithm is technically not limited by system dimensionality, although this factor does affect the amount of computation time.

CONCLUSIONS AND SIGNIFICANCE

The application of a general algorithm for solving singular/bang-bang problems with nonlinear systems is presented. The approach utilizes Pearson apparent linearization of the nonlinear state equations and a limiting process which solves the original problem as a series of nonsingular/nonbang-bang problems. In this work the algorithm is applied to the startup of two CSTR's in series, a problem originally described by Siebenthal and Aris (1964). The Pearson method obtains a good suboptimal estimate of the minimum time and optimal control, but for extremely nonlinear equations, the process can be quite time-consuming. The conjugate gradient (first order) and direct second variation (second order) methods readily refine the suboptimal control to an optimal control, but some care must be exercised in the use of penalty functions for the constraints.

One can conclude, however, that the general algorithm effectively obtains singular/bang-bang control for systems of large state dimension, extreme nonlinearity, and multiple controls. The algorithm handles linear or nonlinear control problems and solves both the fixed and nonfixed final time cases.

The solution of singular/bang-bang problems with nonlinear state equations has been studied by Siebenthal and Aris (1964), Jackson (1966), and Dyson and Horn (1967) using phase plane analysis. Boundary value approximation has been used by Birta and Trushel (1969), and quasilinearization has been applied by Radbill and McCue (1970) to solve bang-bang problems. These methods could be extended to handle singular extremals by using the limiting process studied in this work. Descent methods have been very popular; the works of Ko and Stevens (1971), Seinfeld and Lapidus (1968), Paynter and Bankoff (1966), and Nenonen and Pagurek (1970) exemplify various methods of descent.

A control calculation based on the descent concept generally utilizes a first-order method to start off the computation. This is because the region of convergence of first-order methods is quite large, making a good first guess of the optimal control unnecessary. In contrast, the region of convergence by a second-order method is quite small, so one generally uses the first-order method to obtain a nominal control for the second-order method. Often the differences between the minimized performance indices and the controls generated by the two methods are insignificant, but one cannot predict this sort of information. A second-order method does converge much faster than a

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first-order method in the neighborhood of the optimum, though.

One is not restricted to the use of first-order methods to begin a control calculation. One can use a suboptimal control method, which has the advantage of yielding nearly optimum results with a minimum of computation, to obtain a good control estimate. These methods deliberately approximate the system equations or the optimality conditions. The work of Weber and Lapidus (1971) has shown that the apparent linearization method of Pearson (1962) is an excellent method for obtaining suboptimal control for control constrained nonlinear systems. The Pearson method converts a nonlinear control problem into an equivalent LQP as follows:

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

The solution of an LQP, for the case of singular/bang-bang control, has been discussed by Edgar and Lapidus (1972).

For the constrained equivalent LQP a nested iterative process results for the Pearson method. For a set of assumed state and control trajectories, one satisfies the boundary conditions, the system equations, and the minimization of the Hamiltonian. The entity that is not satisfied is the constraints; the inner iterative process successively penalizes each nonfeasible control until all controls satisfy the constraints to a certain tolerance. The convergence to the constraints is imbedded within the outer iterative process, the approximation of the state equation. The complete process terminates when convergence of the state equation (and state trajectories) is obtained. Therefore this method, although suboptimal, could be classified as an approximation in state space method.

DESCRIPTION OF THE GENERAL ALGORITHM FOR NONLINEAR SYSTEMS

The algorithm for the solution of linear system singular/bang-bang problems has been given in the preceding paper by Edgar and Lapidus. For nonlinear systems, the computational steps are as follows:

Fixed Final Time: Nonlinear State Equation

Step 1: Formulate an analytical apparent linearization by the method of Pearson.

Step 2: Initiate the ϵ limiting process. Set ϵ^i $(i = 0)$. Augment the performance index with $\epsilon^i \int_0^{t_f} \mathbf{u}^T\mathbf{u}\, dt$.

Step 3: Guess the $\mathbf{x}^n$ and $\mathbf{u}^n$ trajectories $(n = 0)$. Calculate $\mathbf{A}^n$ and $\mathbf{B}^n$ $(n = 0)$.

Step 4: Discretize the state equations and performance index. Augment for the constraints, as with linear systems.

Step 5: Use DDP-PF (discrete dynamic programming with penalty functions) to solve the equivalent LQP.

Step 6: If $\|\mathbf{u}^n - \mathbf{u}^{n-1}\| > \gamma$, calculate $\mathbf{A}^{n+1}$, $\mathbf{B}^{n+1}$ based on $\mathbf{u}^n$ and $\mathbf{x}^n$. Return to Step 4. If $< \gamma$, then the converged suboptimal control is obtained. Go to Step 7.

Step 7: Refine the suboptimal control to an optimal one with first-order (if necessary) and second-order descent methods. If $\|\mathbf{u}^0(\epsilon^i) - \mathbf{u}^0(\epsilon^{i-1})\| > \delta$, then update $\epsilon^{i+1} = \alpha\epsilon^i$, $\alpha < 1$. Return to Step 3. If ϵ convergence occurs $(< \delta)$, then the optimal singular/bang-bang control is obtained.

Minimum Final Time: Nonlinear State Equation

Step 1: Guess t_f^i $(i = 1, 2)$.

Step 2: Apply Pearson linearization to obtain the time-varying linear equation. Use DDP-PF in conjunction with the limiting process to obtain the converged suboptimal control as with the fixed final time nonlinear problem.

Step 3: If t_f^i is not the smallest t_f for which all constraints can be met, then generate t_f^{i+1}. Return to Step 2. Otherwise t_f^i is the suboptimal minimum time. Proceed to Step 4.

Step 4: Refine the suboptimal control using first- and second-order methods in conjunction with the limiting process until the optimal control for the specified final time is found.

Step 5: If t_f^i is not the smallest t_f for which all constraints can be met, then generate t_f^{i+1}. Return to Step 4 and restart the limiting process. Otherwise, the minimum time corresponding to singular/bang-bang optimal control is found.

The imbedding of the linear system part of the algorithm into the nonlinear system control calculation (Steps 3 to 6 in the fixed final time nonlinear system computation) is an attractive feature of the general algorithm, even though the resulting control is suboptimal. It also should be noted that for the nonfixed final time case, the same basic approach as that utilized for linear systems is used to obtain the optimal final time and optimal control for nonlinear systems, that is, the nonfixed final time problem is solved as a sequence of fixed final time problems. For linear systems the minimum time is the smallest time for which the control is bang-bang (totally saturated), and the end point constraints are met within a certain tolerance. A method based on the relative degree of saturation of the controls for various final times, presented by Edgar and Lapidus in Part I, is very successful in obtaining the linear system minimum time.

For nonlinear systems this condition must be relaxed somewhat. For a nonlinear minimum time problem the optimal control can contain optimal singular arcs, which are intermediate between the control constraints. These optimal singular arcs do not occur for the linear minimum time problem. Therefore any iteration on the final time (optimal or suboptimal) which is based on the degree of saturation of the control will not always work for nonlinear systems. However, a totally bang-bang control will allow one to use the degree of saturation scheme to obtain the suboptimal minimum time. The minimum time criterion used in this work for optimal or suboptimal methods is the smallest final time for which both the control and end point constraints are met to within a given tolerance. In iterating upon the guessed minimum time, the above criterion determines how close this guess is to the actual minimum time. Because this step yields a suboptimal control, it is unnecessary to obtain a precise estimate of the suboptimal minimum time, since this value is refined in later steps.

The Pearson linearization algorithm used here is very nearly the same one used by Weber and Lapidus to generate suboptimal control. The only major change is in the integration of the state equation. Weber and Lapidus use a Runge-Kutta integration of the full nonlinear equation while this work utilizes the discrete equation

$$\mathbf{x}_{k+1} = \mathbf{\Phi}_k \mathbf{x}_k + \mathbf{\Delta}_k \mathbf{u}_k \qquad (2)$$

for the system integration. $\mathbf{\Phi}_k$ and $\mathbf{\Delta}_k$ are the matrices which represent the continuous nonlinear equation as a time-varying linear discrete equation. This approach yields better results for singular/bang-bang problems than that obtained by Weber and Lapidus' integration scheme.

The descent algorithms tested in this work are the fixed-step gradient method, the steepest descent method, and conjugate gradient method, all first order, and the direct second variation (DSV) method, a second-order

method. These methods are well-documented in the literature; the first-order methods are described in Walder and Storey (1970), and the DSV method is derived in Padmanabhan and Bankoff (1969). These four methods have been combined into a general purpose computer program, but the conjugate gradient and DSV methods are mainly used in this work. The first-order methods require only H_u, while the DSV method utilizes H_u, H_{uu}, H_{ux}, and H_{uz} in the control correction formula.

The most effective formulation for the use of the descent methods is the continuous time formulation, as opposed to the discrete time format used for the DDP-PF algorithm. It is felt that the existence of end point constraints requires accurate integration schemes, and an Eulerian finite difference approximation of the differential equations would necessitate the use of excessive time steps for the integration and other optimization calculations.

AUGMENTING THE CONTINUOUS TIME PROBLEM FOR DESCENT METHODS

The continuous time formulation requires a different penalty function approach than that used for discrete time. The augmenting procedure used by Weber and Lapidus for discrete systems is replaced by one for continuous systems. For end point constraints of the form

$$\mathbf{x}(t_f) = \mathbf{0} \tag{3}$$

the performance index can be augmented with a quadratic term

$$\mathbf{x}^T(t_f)\ \mathbf{S}\ \mathbf{x}(t_f) \tag{4}$$

where S is a diagonal penalty weighting matrix. When the diagonal elements are increased, the final values of the state variables should decrease. One should take care that the continuous time weighting matrices correspond to the same relative weighting used to generate the suboptimal control with the discrete time Pearson method.

For the case of linear inequality constraints

$$\boldsymbol{\alpha}^- \leq \mathbf{u} \leq \boldsymbol{\alpha}^+ \tag{5}$$

one has several alternatives in expressing this in penalty function form. The quadratic form selected here is

$$\int_0^{t_f} [(\mathbf{u} - \boldsymbol{\alpha}^+)^T \boldsymbol{\zeta}\, \mathbf{h}(\mathbf{u} - \boldsymbol{\alpha}^+)\,(\mathbf{u} - \boldsymbol{\alpha}^+) + (\boldsymbol{\alpha}^- - \mathbf{u})^T \boldsymbol{\zeta}\, \mathbf{h}(\boldsymbol{\alpha}^- - \mathbf{u})\,(\boldsymbol{\alpha}^- - \mathbf{u})]\, dt \tag{6}$$

where $\boldsymbol{\zeta}$ is a penalty weighting matrix and $\mathbf{h}(\cdot)$ is a Heaviside step function matrix, with the same requirements as that defined by Weber and Lapidus for inequality constraints. This quantity is then added to the performance index to convert the control constrained problem into an augmented unconstrained control problem, which has an iterative nature. It should be noted that there is no explicit definition of extra state variables with this formulation, as done by Kelley (1962) for continuous time. However, Kelley's formulation is implicit in this augmenting procedure and in the subsequent minimization of the Hamiltonian and the performance index via the minimum principle.

NUMERICAL RESULTS FOR NONLINEAR SYSTEMS

Three numerical examples have been solved in this study using the general algorithm. Only a brief description of the first two examples and their computational results will be given here, but the third example will be presented in detail. Complete information on all three nonlinear problems can be found in Edgar (1971).

The first nonlinear problem solved is the minimum time control of a CSTR with an irreversible, first-order reaction, as described in Lapidus and Luus (1967). The calculated suboptimal minimum time is within 2% of the actual minimum time. The suboptimal control, which is bang-bang, is a good approximation of the optimal control (bang-bang). A number of difficulties are encountered, however, in the total solution of the problem, and they are as follows:

1. The Pearson linearization method requires much computation time, but convergence acceleration schemes do ameliorate this difficulty.
2. The end point penalty function formulation causes the descent method refinement process to be very sensitive to the nominal control and the particular descent technique used; the conjugate gradient method is required to refine the suboptimal control before use of the DSV method.
3. For final times less than the minimum time, allowing control excursions beyond the constraints (oversaturation, as for the DDP-PF method) with the descent methods impedes convergence to the solution.

The second nonlinear problem, which has the maximization of the outlet conversion of a tubular reactor ($A \rightleftarrows B$) as its performance criterion, contains an optimal singular arc and is a fixed final time problem. This problem was also studied by Seinfeld and Lapidus (1968). The solution of this problem demonstrates that:

1. The Pearson method can successfully solve nonlinear problems with a singular arc suboptimally; slight modification of the procedure is required when the state variables are not controllable to the desired steady state in the specified final time.
2. The conjugate gradient method is superior to other first-order methods for computation of singular/bang-bang control. The convergence theory of Johansen (1964) for the method of gradients is computationally verified by the results of this example.

The fact that the conjugate gradient method is the most effective first-order method for singular/bang-bang problems is a direct result of the topography of the iso-Hamiltonian surfaces. This topography consists of long, narrow valleys in function space; optimum step sizes in the search direction alternate between long and short steps. The fixed-step gradient method fails to reach the optimum in a reasonable amount of computing time because of oscillation on the ridges.

Ko and Stevens (1971) have recently proposed a method for singular/bang-bang problems which combines the fixed-step gradient method and an analytical expression for the optimal singular control. Their use of an analytical optimal control has been predicated upon the slow convergence of the fixed-step gradient method for this class of problems. However, the above results show that the use of the fixed-step gradient method here ignores the topography of the problem. Also the derivation of an analytical expression for the optimal singular control requires careful analysis prior to numerical solution; the complexity of the algebra for large dimensions demonstrates that Ko and Stevens' method suffers from the same limitations as phase plane analysis. The general algorithm proposed in this work surmounts this curse of dimensionality, as shown in the following example.

MINIMUM TIME CONTROL OF A TWO-STAGE CSTR

The general algorithm is tested here on a four state variable, two control nonlinear minimum time problem. The system is two nonlinear CSTR's in series with heat

transfer controllers. This system was first suggested by Siebenthal and Aris (1964), but they could not solve it due to the limitations of phase plane analysis. The description of the dimensionless normalized system is as follows:

$$dx_1/dt = -x_1/\mu + R_1(x_1, x_2) \quad (7)$$

$$dx_2/dt = -(\mu\gamma_1 + 1.0 - \mu)x_2/\mu + R_1(x_1, x_2) - (x_2 + \eta_1)u_1 \quad (8)$$

$$dx_3/dt = 1.0/(1.0 - \mu)\ (\lambda x_1 - x_3) + R_2(x_3, x_4) \quad (9)$$

$$dx_4/dt = -1.0/(1.0 - \mu)\ [-\lambda x_2 + x_4\ ((1.0 - \mu)\gamma_2 + \mu)] + R_2(x_3, x_4) - (x_4 + \eta_2)\ u_2 \quad (10)$$

where x_1 and x_3 are normalized concentration variables, x_2 and x_4 are normalized temperature variables, μ is a residence time term, λ is the fraction of feed going to the first reactor, and γ_i and η_i are constants arising out of heat transfer terms. The two normalized controls are u_1 and u_2, and they have cooling capacity only. The normalized reaction rate term $R(x_i, x_{i+1})$ is for a first-order reversible reaction, $A \rightleftarrows B$.

A set of final and initial operating conditions that yield optimal singular behavior for the minimum time problem are as follows:

1. Final condition: As shown by Siebenthal and Aris, a final condition where $\partial R/\partial T = 0$ (T = temperature) may yield optimal singular arcs for the two state variable (single CSTR) problem with a reversible reaction. Therefore this type of final condition is selected for both reactors. This particular boundary condition is an important steady state, since at this point the reaction rate is maximized with respect to the temperature. So the final steady state temperatures, concentrations, and controls can be found by solving simultaneously four steady state equations ($= 0$) and two maximization conditions ($\partial R/\partial T = 0$). Using this data one obtains the normalized Equations (7) to (10).

2. Initial condition: It is assumed that both reactors are initially at the steady state temperature of reactor 2. This can be obtained by a heating coil used only for startup situations. The reaction $A \rightleftarrows B$ is at equilibrium in each reactor.

Therefore the boundary conditions for this problem are

$$\mathbf{x}(t_f) = \mathbf{0} \quad \mathbf{x}^T(0) = [0.1962 \quad -0.0372 \quad 0.0946 \quad 0.0] \quad (11)$$

The numerical values of the parameters are as follows:

$$\lambda = 0.5 \qquad \gamma_1 = 9.1558 \quad \eta_1 = 0.1592$$

$$\mu = 0.3333 \quad \gamma_2 = 4.4385 \quad \eta_2 = 0.122$$

The normalized controls are bounded as follows:

$$-8.1558 \leq u_1 \leq 8.1558 \qquad -3.4385 \leq u_2 \leq 3.4385 \quad (12)$$

The lower bound corresponds to adiabatic operation. The dimensionless and normalized reaction rates are as follows:

$$R_1(x_1, x_2) = 1.5 \times 10^7\ (0.5251 - x_1)\ \exp(-10/(x_2 + 0.6932)) - 1.5 \times 10^{10}\ (x_1 + 0.4748)\ \exp(-15/(x_2 + 0.6932)) - 1.4280 \quad (13)$$

$$R_2(x_3, x_4) = 1.5 \times 10^7\ (0.4236 - x_3)\ \exp(-10/(x_4 + 0.6460)) - 1.5 \times 10^{10}\ (x_3 + 0.5764)\ \exp(-15/(x_4 + 0.6560)) - 0.5086 \quad (14)$$

TABLE 1. COEFFICIENT MATRICES $\mathbf{A}(t)$ AND $\mathbf{B}(t)$ FOR PEARSON LINEARIZATION OF TWO CSTR'S IN SERIES

$$A_{11} = -3.0 - 1.5 \times 10^7 \exp[-10/(x_2 + 0.6932)] - 1.5 \times 10^{10} \exp[-15/(x_2 + 0.6932)]$$

$$A_{21} = A_{11} + 3.0; \quad A_{31} = 0.75; \quad A_{41} = 0.0$$

$$A_{12} = \{(0.5252)\ (1.5 \times 10^7) \exp[-10/(x_2 + 0.6932)] - (0.4748)\ (1.5 \times 10^{10}) \exp[-15/(x_2 + 0.6932)] - 1.4280\}/x_2$$

$$A_{22} = A_{12} - 11.17; \quad A_{32} = 0.0; \quad A_{42} = 0.75$$

$$A_{13} = 0.0; \quad A_{23} = 0.0; \quad A_{43} = 1.5 + A_{33}$$

$$A_{33} = -1.5 - 1.5 \times 10^7 \exp[-10/(x_4 + 0.6560)] - 1.5 \times 10^{10} \exp[-15/(x_4 + 0.6560)]$$

$$A_{14} = 0.0; \quad A_{24} = 0.0; \quad A_{44} = A_{34} - 4.9385$$

$$A_{34} = \{(0.4236)\ (1.5 \times 10^7) \exp[-10/(x_4 + 0.6560)] - (0.5764)\ (1.5 \times 10^{10}) \exp[-15/(x_4 + 0.6560)] - 0.5086\}/x_4$$

$$\mathbf{B} = \begin{Bmatrix} 0 & 0 \\ -(x_2 + 0.1592) & 0 \\ 0 & 0 \\ 0 & -(x_4 + 0.1220) \end{Bmatrix}$$

Further information on the selection of parameters, the calculation of steady states, and the normalization of the system can be found in Edgar (1971).

PEARSON LINEARIZATION OF THE SYSTEM EQUATIONS

The coefficient matrices obtained from the Pearson linearization of the system are given in Table 1. Note that A_{12}, A_{22}, A_{34}, and A_{44} have the possibility of becoming unbounded for x_2 or $x_4 = 0$. However, the fractions with x_2 or x_4 in the denominator approach a limit of zero as x_2 or x_4 approaches zero. This limit is related to the fact that

$$\partial R_1/\partial x_2 = 0 \quad \text{at} \quad x_2 = 0 \quad \partial R_2/\partial x_4 = 0 \quad \text{at} \quad x_4 = 0 \quad (15)$$

In order to obtain a first estimate of the minimum time, the system is integrated with $u_i(t) = 0.0$ ($i = 1, 2$). Since this control vector is the final steady state control vector, and there is only one steady state for this control vector, then the state variables will eventually go to the origin, the final steady state. This gives one an idea of the time scale of the process. Using this data, a first guess of $t_f = 1.0$ is made, and the Pearson method obtains definitely unsaturated suboptimal controls. Subsequent guesses on the final time are 0.5, 0.375, 0.356. u_1 is mainly unsaturated for these final times, but u_2 becomes almost totally bang-bang for $t_f = 0.356$.

For $t_f < 0.356$ the suboptimal controls become oversaturated, which indicates that the origin is unreachable for the postulated final time. For all final times greater than 0.356, convergence to the state equation is difficult to attain without excessive amounts of computer time, which does not occur for the other nonlinear problems solved in Edgar (1971). This is due to the extreme nonlinearity of the state equations and the resulting high sensitivity of the coefficient matrices $\mathbf{A}(\mathbf{x})$ and $\mathbf{B}(\mathbf{x})$ to the assumed state trajectory. For successive iterations oscillation of the computed controls is observed, and an averaging process from one iteration to the next can be instituted

to speed up convergence to the state equation. u_1 shows the most variation, while u_2 remains fairly constant during the approximation of the state equation. The suboptimal minimum time of 0.356 is used to initiate the refinement process in the following section.

DESCENT METHOD RESULTS

The problem is formulated with continuous penalty functions for the control constraints and end point constraints and the quadratic control integral for the limiting process ($\epsilon \rightarrow 0$). The resulting performance index is

$$J_c = \int_0^{t_f} dt + \epsilon \int_0^{t_f} \mathbf{u}^T \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \mathbf{u}\, dt + \mathbf{x}^T(t_f)\, \mathbf{S}\, \mathbf{x}(t_f) + \int_0^{t_f} [(\mathbf{u} - \boldsymbol{\alpha}^+)^T \boldsymbol{\zeta}\, \mathbf{h}(\mathbf{u} - \boldsymbol{\alpha}^+)(\mathbf{u} - \boldsymbol{\alpha}^+) + (\boldsymbol{\alpha}^- - \mathbf{u})^T \boldsymbol{\zeta}\, \mathbf{h}(\boldsymbol{\alpha}^- - \mathbf{u})(\boldsymbol{\alpha}^- - \mathbf{u})]\, dt \quad (16)$$

where

$$\boldsymbol{\alpha}^+ = \begin{bmatrix} 8.1558 \\ 3.4385 \end{bmatrix} \quad \text{and} \quad \boldsymbol{\alpha}^- = -\boldsymbol{\alpha}^+ \quad (17)$$

The adjoint equations for this system are very complex, and they can be found in Edgar (1971). The two important partial derivatives of the Hamiltonian are for unsaturated control (control penalty function terms are zero)

$$H_{u_1} = -z_2(x_2 + 0.1592) + 2\epsilon u_1 \quad (18)$$

$$H_{u_2} = -z_4(x_4 + 0.122) + 2\epsilon u_2 \quad (19)$$

Other derivatives (H_{uu}, H_{ux}, H_{uz}) can be found in Edgar.

For the suboptimal minimum time and $\epsilon = 10^{-8}$, the descent methods yield an optimal control which indicates that the actual minimum time is less than $t_f = 0.356$, due to satisfaction of the end point constraints and unsaturation of u_1 and u_2. 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. Therefore the estimate of the minimum time is successively reduced (0.350, 0.346, 0.342) and the limiting process ($\epsilon \rightarrow 0$) applied to obtain the optimal singular/bang-bang control. The limiting process consists of solving the problem for three values of ϵ: 10^{-4}, 10^{-6}, 10^{-8}.

The final time of 0.342 satisfies the criterion for the minimum time (satisfaction of the end point and control constraints), and the optimal controls (u_1 and u_2) calculated by the conjugate gradient/DSV methods for various stages of the limiting process are shown in Figures 1 and 2. There is a different effect of the reduction of ϵ on u_1 and u_2, since $u_1 \leq 8.1558$ and $u_2 \leq 3.4385$. The optimal control (u_2) for $\epsilon = 10^{-5}$ is shown in Figure 2, although this particular ϵ is not used in the limiting process. The number of iterations required for convergence of the descent methods decreases significantly for larger ϵ. This is a validation of the convergence theory of Johansen (1964).

For the minimum time of 0.342 the control sequences for the optimal singular/bang-bang control ($\epsilon = 10^{-8}$) are

u_1	u_2
adiabatic (0.0069)	adiabatic (0.0147)
full cooling (0.0745)	full cooling (0.1361)
adiabatic (0.1986)	adiabatic
singular	

The estimated switching times are given in parentheses.

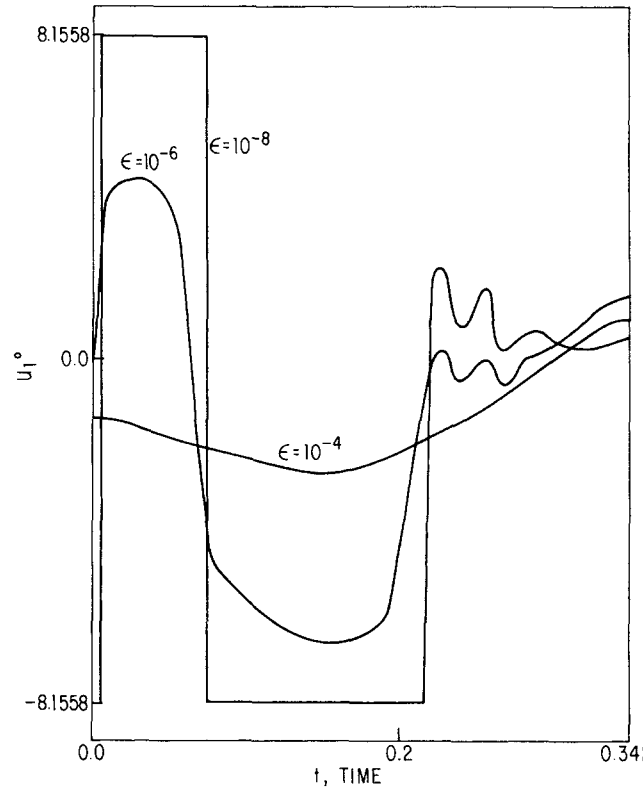

Fig. 1. Optimal u_1 for various values of ϵ, two-stage CSTR $t_f = 0.342$; $\tau = 0.00342$; $\zeta = 100$; $\epsilon = 10^{-4}, 10^{-6}, 10^{-8}$; $S = I_4$.

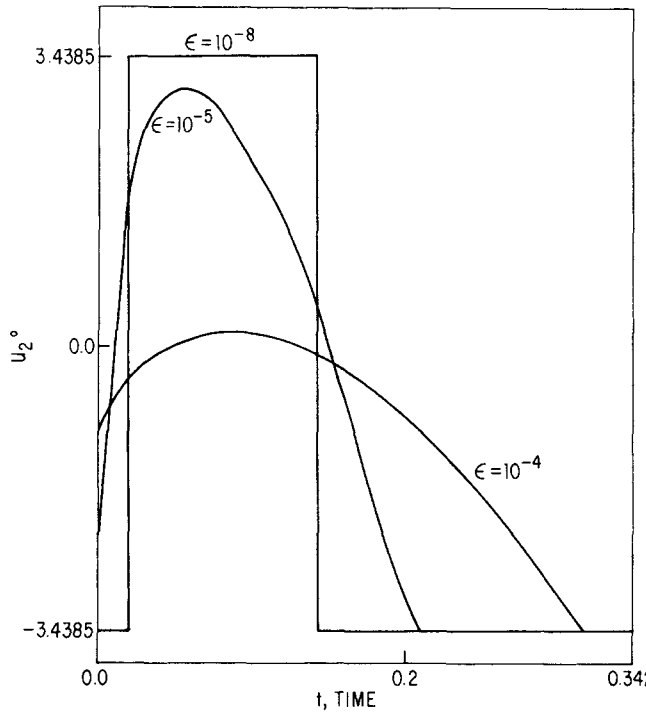

Fig. 2. Optimal u_2 for various values of ϵ, two-stage CSTR $t_f = 0.342$; $\tau = 0.00342$; $\zeta = 100$; $\epsilon = 10^{-4}, 10^{-5}, 10^{-8}$; $S = I_4$.

These times are estimated by a formula given in the preceding work.

For the case $\epsilon = 10^{-8}$ modification of the descent algorithm has to be made to obtain meaningful results. For all linear and nonlinear minimum time problems solved previously in this study, equal weighting of the various final value penalty functions yields final states which are

within a certain numerical tolerance, for example, 10^{-4} of the origin. In other words S the penalty matrix in Equation (4) is usually selected as $\mathbf{S} = s \cdot \mathbf{I}_n$ where n is the number of linear end point constraints handled by penalty functions, s is a scalar weighting factor, and $\mathbf{I}_n$ is the $n \times n$ identity matrix. For this problem it is necessary to vary the diagonal components of S in order to have each final state satisfy some tolerance. Analytically this corresponds to a final value criterion of

$$\min_{s_{jj}} \max_{i} |x_i(t_f)|$$

Using equal weighting for the components of S results in $|x_2(t_f)| < 10^{-5}$ while $|x_3(t_f)| > 0.0025$. By adjusting the penalty weighting coefficients proportionally to the final state values obtained for equal weighting, the following weighting coefficients and end point values result:

$$S_{11} = 1.2 \qquad x_1(t_f) = -0.00171$$

$$S_{22} = 0.003 \qquad x_2(t_f) = +0.00103$$

$$S_{33} = 2.0 \qquad x_3(t_f) = +0.00173$$

$$S_{44} = 1.1 \qquad x_4(t_f) = -0.00169$$

It is interesting to compare the results for the limiting singular/bang-bang case for this four state variable problem with those of Siebenthal and Aris (1964) for the two state variable problem. For equilibrium initial conditions analogous to this example, Siebenthal and Aris have shown that the optimal control is bang-bang. However, there is more than one bang-bang approach to the origin, and further analysis is required to find the optimal control. For the four state variable problem u_2 is indeed bang-bang, but u_1 exhibits an optimal singular arc. Therefore one sees that it is very difficult to extend results from the phase plane to higher dimensional problems.

The DSV method, when used to improve upon the conjugate gradient results, does not change the computed control appreciably. For the total solution of the problem, the Pearson linearization process requires 130 seconds (IBM 360/91) to obtain the suboptimal minimum time and control estimate. The refinement of these two entities via the limiting process and descent methods takes another 110 seconds; a total of four minutes is required to obtain the final singular/bang-bang solution.

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NOTATION

$\mathbf{A}$ = matrix
$\mathbf{B}$ = matrix
d = parameter
$\mathbf{h}$ = Heaviside step function matrix
H = Hamiltonian
$\mathbf{I}_n$ = $n \times n$ identity matrix
J = performance index
N = number of discrete steps of control
$\mathbf{Q}$ = matrix
$\mathbf{R}$ = matrix
R = reaction rate term
s = parameter
$\mathbf{S}$ = matrix
t = time
T = temperature
$\mathbf{u}$ = control vector
$\mathbf{x}$ = state vector
$\mathbf{z}$ = adjoint vector

Greek Letters

α = control bound; α^+ = upper bound, α^- = lower bound
$\boldsymbol{\Delta}$ = matrix
ϵ = parameter in limiting process
$\boldsymbol{\Gamma}$ = matrix
$\boldsymbol{\Phi}$ = matrix
τ = discrete time sampling interval
$\boldsymbol{\zeta}$ = control penalty weighting coefficient

Subscripts

f = final (time)
i, j = matrix or vector component
k = discrete time step index
min = minimum (time)
$\mathbf{u}$ = partial derivative with respect to $\mathbf{u}$
$\mathbf{x}$ = partial derivative with respect to $\mathbf{x}$
$\mathbf{z}$ = partial derivative with respect to $\mathbf{z}$

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