

- Meyer, W., and P. K. Shen, "Separation and Purification by Continuous Countercurrent Crystallization," paper presented at 64th AIChE National Meeting (1969).
- Moyers, Jr., C. G., "Macroscopic Characteristics of a Continuous Center-Feed Column Crystallizer," Ph.D. thesis, Univ. Delaware, Newark (1971).
- , "Process for Purification by Crystallization," U.S. Patent No. 3,796,060 (March 12, 1974).
- Mullin, J. W., *Crystallization*, Butterworths, London (1961).
- Player, M. R., "Mathematical Analysis of Column Crystallizers," *Ind. Eng. Chem. Process Design Develop.*, 8, 210 (1969).
- Powers, J. E., "Column Crystallization: Phenomenological Theory," in *Symp. über Zonenschmelzen und Kalonnenkristallisation*, H. Schildknecht (ed.), Karlsruhe (1963).
- Ritter, D. L., "Washing of Brine from Ice Crystals by Counter-current Flow," Ph.D. thesis, Mass. Inst. Technol., Cambridge (1969).
- Schildknecht, H., and H. Vetter, "Über das kontinuierliche Kolonnenkristallisieren," *Angew. Chem.*, 73, 612 (1961).
- Schildknecht, H., and K. Mass, "Kolonnenkristallisieren," *Warne*, 69, 121 (1963).
- Timmermans, J., *Physico-Chemical Constants of Pure Organic Compounds*, Elsevier, New York (1950).
- Yagi, S., H. Inoue, and H. Sakamoto, "Investigation of Countercurrent Crystallization Purification Apparatus," *Kagaku Kagaku*, 72, 415 (1963).
- Zief, M., and W. R. Wilcox, *Fractional Solidification*, Vol. 1, Marcel Dekker, New York (1967).

Manuscript received February 12, 1974; revision received August 5 and accepted August 6, 1974.

# On the Optimization of Distributed Parameter Systems with Boundary Control: A Counter Example for the Maximum Principle

A counterexample is given to the strong maximum principle for boundary control of a class of distributed parameter systems. The particular system deals with chemical reactors suffering catalyst decay and is in the class whose members are described by sets of first-order partial differential equations of the hyperbolic type. It is shown that an optimal control exists and that over any finite time interval in which the control is unconstrained the exit conversion from the reactor remains constant. It is further shown that for certain values of the parameters the optimal control policy violates the necessary conditions of the strong maximum principle for boundary control of distributed parameter systems.

**F. GRUYAERT  
and  
C. M. CROWE**

Department of Chemical Engineering  
McMaster University  
Hamilton, Ontario, Canada

## SCOPE

The maximum principle of Pontryagin (1962) has been used extensively in the optimal control of lumped parameter systems described by ordinary differential equations. A similar strong maximum principle was developed by Degtyarev and Sirazetdinov (1967) for the optimal control of distributed parameter systems described by a set of first-order partial differential equations and where the control was distributed. For the case of boundary control, where the control enters in the boundary conditions to the partial differential equations or where the control is a function of one independent variable only, Degtyarev and Sirazetdinov obtained a weaker form of the necessary conditions. Whereas in the case of distributed control, the

hamiltonian must reach a maximum with respect to the control at the optimum, the boundary hamiltonian, in the case of boundary control, need only remain stationary with respect to the control at the optimum whenever the control is unconstrained. However, several authors have also stated the strong maximum principle as a necessary condition for optimality in the boundary control case.

In the present study, the validity of this strong maximum principle will be examined for a certain class of boundary control problems. The particular example under investigation relates to the optimal inlet temperature control of a tubular fixed-bed chemical reactor with slowly decaying catalyst.

## CONCLUSIONS AND SIGNIFICANCE

For particular values of the parameters in the partial differential equations describing the reactor system, the strong maximum principle for boundary control requires the optimal control to be totally constrained.

By considering a quasi steady state approximation, an equivalent lumped parameter system can be formulated and Pontryagin's Maximum Principle can be applied. Existence of an optimal controller in the lumped formulation is shown and the optimal control policy can be determined as a unique Pontryagin policy. For certain values of the parameters, it is shown that a totally constrained policy cannot be optimal. The optimal control policy then clearly violates the necessary conditions of the strong maximum principle for boundary control in the distributed form of the problem. It is further proved that if the

optimal control policy contains an unconstrained part over any finite time interval, the exit conversion from the reactor then remains constant over that time interval. A numerical example, where the optimal control policy is unconstrained for a finite time interval, also shows the constant exit conversion property at the optimum.

If the quasi steady state approximation cannot be used, the distributed problem cannot be lumped and an existence proof of an optimal controller in the class of piecewise continuous functions cannot easily be found. Numerical results for this case, however, support our findings derived for the lumpable problem.

A strong maximum principle should therefore not be used as a necessary condition for optimality of boundary control in this class of distributed parameter problems.

In recent years, much research has been done on the optimal control of distributed parameter systems, described by sets of simultaneous partial differential equations. Necessary conditions for optimality have been derived in the form of various maximum principles.

A strong form of the maximum principle, requiring that the hamiltonian reach its absolute maximum with respect to the control vector at the optimum, has been derived by Degtyarev and Sirazetdinov (1967) for the optimal control of a system of simultaneous first-order partial differential equations where the control is distributed. A similar form of the maximum principle was proved independently by Chang (1967). In both approaches, the distributed control vector is sought in the class of piecewise continuous functions with a finite number of lines of discontinuity and such that finite limits for the value of the control exist at both sides of a line of discontinuity.

Degtyarev and Sirazetdinov (1967) also derived necessary conditions for optimality of distributed systems with boundary control.\* This results in a weak maximum principle, requiring that the boundary hamiltonian remain stationary with respect to the control at the optimum whenever the control is in the interior of the admissible control region (unconstrained) and that it reach a local maximum when the control is at the boundary of the admissible control region (constrained). A similar result was also obtained by Ogunye and Ray (1971a,b), but the authors express some doubt that the strong form of the maximum principle is a necessary condition for the boundary control case.

A strong maximum principle for the boundary control of distributed parameter systems has been stated from time to time in the literature. The requirement of a strong maximum principle to be a necessary condition for optimality of boundary control in hyperbolic distributed parameter systems has been claimed by Chang and Bankoff (1969), Tarassov, Perlis, and Davidson (1969), and very recently also by Holliday and Storey (1973).

The proofs given by Chang (1967) and by Tarassov

(1968) for the boundary control case are both based by analogy on those for the distributed control problem.

In the derivation given by Holliday (1972), the author comes to the conclusion of a strong maximum principle, for both distributed and boundary control of parabolic and hyperbolic systems, through a first-order perturbation analysis.

A similar theorem can be found in the book by Butkovskii (1969), but the proof is missing.

The strong maximum principle for boundary control was also stated without proof by Nishida, Ichikawa, and Tazaki (1972) and by Davis and Perkins (1972). However, these authors did not use the second derivative condition for the boundary hamiltonian in their computational work.

The maximum principle for boundary control, as it can be found in the literature, will be formulated. An optimal control problem, which is related to fixed-bed tubular reactors with decaying catalyst, will be presented. Existence of an optimal boundary control policy will be shown and properties of the optimal policy will be derived. A whole class of problems, where the strong maximum principle for boundary control fails to provide us with necessary conditions, will be identified.

### STATEMENT OF THE MAXIMUM PRINCIPLE FOR BOUNDARY CONTROL

Consider the class of systems where the state equations are given by a set of simultaneous first-order partial differential equations (PDE):

$$v_t = F(z, t, v, v_z, u) \quad (1)$$

where

$$v \in R^n, \quad u \in R^m$$

and

$$F_i = F_i^0(z, t, v, u) + F_i^1(z, t, u) v_{iz} \quad i = 1, 2, \dots, n \quad (2)$$

The subscripts  $t$  and  $z$  in (1) and (2) refer to partial derivation with respect to the independent variables  $t$  and  $z$ . The vector-valued function  $F$  is defined on the rectangle  $[z_0, z_f] \times [t_0, t_f]$  and is assumed to be at least twice piecewise continuously differentiable with respect to its arguments. The vector  $u(t)$  is a bounded piecewise continuous boundary control on  $[t_0, t_f]$  and  $u \in U$  where  $U$  is an admissible control region in  $R^m$ .

The initial and boundary conditions for the state vector  $v$  are given by two vector-valued functions with piecewise continuous second derivatives:

\* The term *boundary control* is used here, both for those control variables which appear explicitly in the initial or boundary conditions of the state equations and for those control variables which appear in the state equations as a function of one independent variable only. This latter case, also called *uniform control*, defines a proper subset of the *boundary controls* since one can always introduce additional differential equations in these variables with new control variables in the initial or boundary conditions to these differential equations.

$$v(z_0, t) = \alpha(t); \quad v(z, t_0) = \beta(z) \quad (3)$$

The objective function is given by

$$P = \int_{t_0}^{t_f} \int_{z_0}^{z_f} F_0(z, t, v, v_z, u) dz dt \quad (4)$$

where

$$F_0 = F_0^0(z, t, v, u) + \sum_{j=1}^n F_0^j(z, t, u) v_{jz} \quad (5)$$

The optimal boundary control problem can then be formulated as: among all admissible controls defined on  $[t_0, t_f]$ , find a control  $u(t)$  with  $t \in [t_0, t_f]$  such that the functional  $P$  attains its maximum value.

A hamiltonian function  $H$  is introduced by

$$H(z, t, v, v_z, u) = F_0 + \langle \lambda, F \rangle \quad (6)$$

where the adjoint vector  $\lambda$  is given by

$$\frac{\partial \lambda}{\partial t} = -\nabla_v H + \frac{\partial}{\partial z} (\nabla_{v_z} H) \quad (7)$$

subject to the following terminal and boundary conditions:

$$\lambda|_{t=t_f} = 0; \quad \nabla_{v_z} H|_{z=z_f} = 0 \quad (8)$$

The inner product  $\langle, \rangle$  used in (6) is defined as the scalar product between two vectors and the notation  $\nabla$  is used to indicate the gradient operator.

Since the control  $u(t)$  is a function of one independent variable only, a boundary hamiltonian  $\bar{H}$  is defined as

$$\bar{H} = \int_{z_0}^{z_f} H dz \quad (9)$$

An admissible control  $u^+(t)$  is said to satisfy the maximum condition in  $\bar{H}$  if at any  $t \in [t_0, t_f]$ , the function  $\bar{H}$  attains its absolute maximum with respect to all admissible controls, that is,

$$\bar{H}(t, v^+, v_z^+, u^+) = \sup_{u \in U} \bar{H}(t, v^+, v_z^+, u) \quad (10)$$

The maximum principle for boundary control, as can be found in the literature referred to above, states then:

For an admissible control  $u^+(t)$  to be optimal with respect to the performance index  $P$ , it is necessary that  $u^+(t)$  satisfy the maximum condition in  $\bar{H}$  almost everywhere on  $[t_0, t_f]$ .

## A BOUNDARY CONTROL PROBLEM

We consider a specific problem described by

$$\frac{\partial x}{\partial z} = K(k)(1-x)\psi \quad (11)$$

$$\frac{\partial \psi}{\partial t} = -k(1-x)^r \psi \quad (12)$$

where  $x(z, t)$  and  $\psi(z, t)$  are the distributed state variables and  $k(t)$  is a boundary control. The independent variables  $z$  and  $t$  are normalized:  $z \in [0, 1]$ ,  $t \in [0, 1]$ .

The functional  $K(k)$  is given by

$$K = Ak^p \quad (13)$$

where  $A$  and  $p$  are positive parameters. The admissible control region is defined as

$$U = \{k | k_* \leq k(t) \leq k^*\} \quad (14)$$

Initial and boundary conditions to the PDE (11) and

(12) are specified as

$$x(0, t) = x_0(t); \quad \psi(z, 0) = \psi_0(z) \quad (15)$$

where  $x_0(t)$  and  $\psi_0(z)$  are piecewise continuous and

$$0 \leq x_0(t) \leq 1; \quad 0 < \psi_0(z) < \infty$$

The optimal control problem is then to find a piecewise continuous control  $k(t) \in U$  which maximizes the objective function  $P$  over all admissible controls, where  $P$  is defined as

$$P = \int_0^1 [x(1, t) - x_0(t)] dt \quad (16)$$

## Remark

This example is particular in the sense that in the domain of definition the characteristic lines of the PDE are orthogonal and parallel to the coordinate axes  $z$  and  $t$ . This problem therefore does not fully comply with the conditions for the use of the maximum principle as formulated by Chang, Tarassov, and Butkovskii. This discrepancy can be resolved by reformulating our state equations (11) to (12) as

$$\frac{\partial x}{\partial t} = \frac{1}{\epsilon} \left( K(k)(1-x)\psi - \frac{\partial x}{\partial z} \right) \quad (17)$$

$$\frac{\partial \psi}{\partial t} = -k(1-x)^r \psi - \epsilon \frac{\partial \psi}{\partial z} \quad (18)$$

where the parameter  $\epsilon$  is positive and can be chosen as small as possible.

The characteristics are then straight lines in the  $z \times t$  domain which for small values of  $\epsilon$  form angles of the order of  $\epsilon$  radians with respect to the  $z$  and  $t$  axes, respectively. The ordinary differential equations which describe the system along the characteristics then have the same right-hand side expressions as Equations (11) and (12).

Initial and boundary conditions to (17) and (18) can be chosen as

$$\begin{aligned} x(0, t) &= \begin{cases} x_0(t) & \text{for } t \in [0, 1 - \epsilon] \\ 1 & \text{for } t \in (1 - \epsilon, 1] \end{cases}; \\ x(z, 0) &= 1 \quad \text{for } z \in [0, 1] \\ \psi(0, t) &= 0 \quad \text{for } t \in [0, 1]; \\ \psi(z, 0) &= \begin{cases} \psi_0(z) & \text{for } z \in [0, 1 - \epsilon] \\ 1 & \text{for } z \in (1 - \epsilon, 1] \end{cases} \end{aligned} \quad (19)$$

The particular problem with orthogonal characteristics is the limit case of a sequence of problems with skewed characteristics as  $\epsilon \rightarrow 0$ . Moreover, one would reasonably expect that the value of the objective function, for a particular control  $k(t)$  in the skewed problem, will converge smoothly to the value of  $P$  in the orthogonal problem, with the same control policy as  $\epsilon \rightarrow 0$ .

## ANALYSIS OF THE PROBLEM

### The Maximum Principle for Boundary Control

Proceeding with the investigation of the problem with orthogonal characteristics, we define a hamiltonian function  $H$  as

$$H = \lambda K(k)(1-x)\psi - \mu k(1-x)^r \psi \quad (20)$$

where the adjoint variables  $\lambda$  and  $\mu$  are given by

$$\frac{\partial \lambda}{\partial z} = -\frac{\partial H}{\partial x}; \quad \frac{\partial \mu}{\partial t} = -\frac{\partial H}{\partial \psi} \quad (21)$$

with terminal and boundary conditions

$$\lambda(1, t) = 1; \quad \mu(z, 1) = 0 \quad (22)$$

The boundary hamiltonian  $\bar{H}$  is defined as in (9).

It is possible to prove analytically (Appendix A) that for all values of the parameter  $p$  greater than 1 the boundary hamiltonian  $\bar{H}$  is a strictly convex function of  $k$ . Hence  $\bar{H}$  attains its absolute maximum with respect to  $k$  either at  $k_*$  or  $k^*$ . If an optimal admissible control  $k^+(t)$  exists in the class of piecewise continuous functions, the strong maximum principle for boundary control then requires that the optimal control be piecewise continuous and constrained almost everywhere on the time domain  $t \in [0, 1]$ .

#### EQUIVALENT LUMPED PARAMETER SYSTEM

By introducing a new state variable  $\phi(t)$  defined as

$$\phi(t) = \int_0^1 \psi(z, t) dz \quad (23)$$

and letting  $x_0(t) = 0$  for convenience, the problem (11), (12), and (15) can be written as

$$\max P = \max_{k(t) \in U} \int_0^1 f_0(\phi, k) dt \quad (24)$$

$$\frac{d\phi}{dt} = f_1(\phi, k) \quad (25)$$

with the initial condition

$$\phi(0) = \phi_0 = \int_0^1 \psi_0(z) dz \quad (26)$$

The functions  $f_0$  and  $f_1$  will be referred to as 'velocities' and are given by

$$f_0 = 1 - \exp(-K(k)\phi) \quad (27)$$

$$f_1 = \frac{-k}{rK(k)} (1 - \exp(-rK(k)\phi)) \quad (28)$$

The extended velocity set  $\hat{V}(\phi)$ , as used by Lee and Markus (1967), is defined as

$$\hat{V}(\phi) = \{f_0(\phi, k), f_1(\phi, k) | k_* \leq k \leq k^*\} \quad (29)$$

and is given in Figure 1 for certain values of  $\phi$  and a specified set of parameter values and control constraints. The velocity line for a fixed  $\phi$  has a sigmoid shape in general but loses its inflection point for small values of  $\phi$ .

#### EXISTENCE OF AN OPTIMAL CONTROLLER

Since  $\hat{V}(\phi)$  is not a convex set with regard to the admissible control values  $k$ , we introduce the concept of a relaxed (or chattering) control. A relaxed controller, which can be seen as the limit of very fast switching between two or more admissible control policies, has been treated extensively in the literature (Warga, 1962; McShane, 1967a,b; Lee and Markus, 1967; Horn and Bailey, 1968; Bailey, 1974; Fjeld, 1974).

The main importance of a relaxed controller for our problem is that every point  $(f_0, f_1)$  in the convex hull of the set  $\hat{V}(\phi)$  can be reached. Since the relaxed controllers include the classical control policies  $k(t) \in U$  as a subset, we will denote the controls which correspond to points  $(f_0, f_1) \in \hat{V}(\phi)$  as classical controllers and those cor-

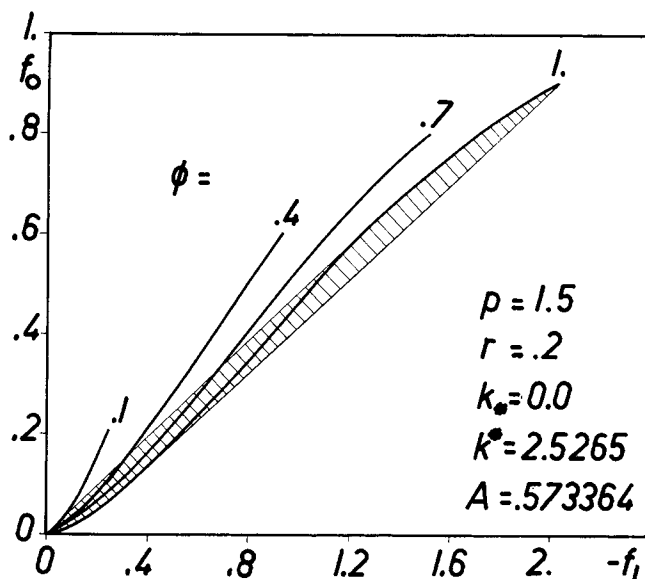


Fig. 1. Extended velocity set  $\hat{V}(\phi)$  and  $\text{co } \hat{V}(\phi)_{\phi=1.0}$ .

responding to points  $(f_0, f_1) \in \text{co } \hat{V}(\phi)$  but  $\notin \hat{V}(\phi)$  as pure relaxed controllers.

Existence of an optimal relaxed controller for our problem (24) to (28) can then be asserted by appeal to a proof given by Lee and Markus (1967; Theorem 5, pp. 271-273).

#### Pontryagin's Maximum Principle

A hamiltonian function  $H_l$  for the lumped parameter system (24) to (28) is defined as

$$H_l = f_0 + \gamma f_1 \quad (30)$$

with the adjoint equation

$$\frac{d\gamma}{dt} = - \frac{\partial H_l}{\partial \phi} \quad (31)$$

and

$$\gamma(1) = 0 \quad (32)$$

An optimal relaxed control policy then satisfies the classical Maximum Principle (Pontryagin et al., 1962; McShane, 1967b). The corresponding value of the hamiltonian  $H_l^+$ , which remains constant almost everywhere on the time domain, is given by

$$H_l^+ = H_l^+|_{t=1} = f_0(\phi(1), k^*) \quad (33)$$

and is strictly positive for all problems with a finite final time.

By rearranging (30) as follows:

$$f_0 = H_l + \gamma(-f_1) \quad (34)$$

the value of the hamiltonian  $H_l$  is the intercept of the  $f_0$  axis with a hamiltonian line going through a point  $(f_0 - f_1)$  with slope  $\gamma$  (Figure 2). For an optimal control policy, it is necessary, in order to maximize  $H_l$ , that for any fixed value of  $\phi$ , the point (or points) of support  $(f_0, -f_1) \in \text{co } \hat{V}$  and lying on the hamiltonian line, correspond either to the uppermost extreme point of  $\text{co } \hat{V}$  (where  $k = k^*$ ) and/or the point (or points) of tangency of a hamiltonian line with slope  $\gamma$ , which is tangent from above to the convex hull of the velocity set.

Furthermore, all hamiltonian lines, corresponding to different values of  $\phi$ , have the point  $H_l^+$  on the  $f_0$  axis

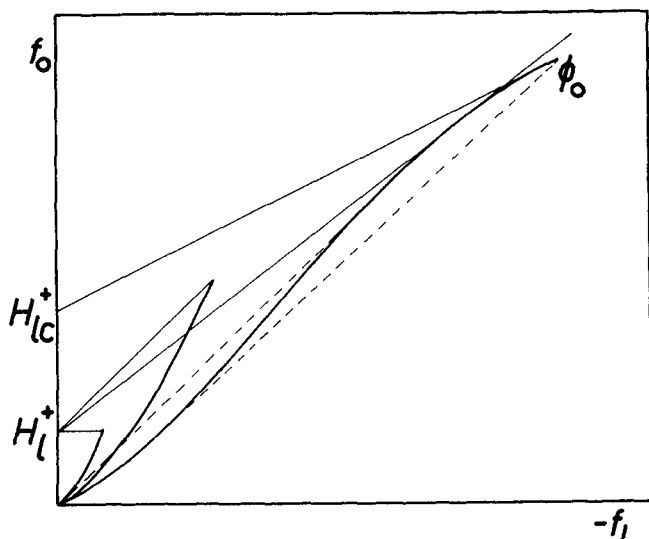


Fig. 2 Extended velocity set  $\hat{V}(\phi)$  and hamiltonian lines  $f_0 = H_l + \gamma(-f_1)$ .

in common for the optimal control policy. Since  $H_l^+ > 0$  and through the geometry of  $\text{co } \hat{V}(\phi)$ , the point of support  $(f_0, -f_1)$  for any given value of  $\phi$  is unique and belongs to the velocity set  $\hat{V}(\phi)$  itself. The corresponding optimal controller is therefore a classical controller. Since both  $f_0$  and  $f_1$  are continuous functions of  $\phi$  and  $k$ , for  $k \in U$ , the optimal controller  $k^+(t)$  will also be a continuous function and hence belongs to the class of piecewise continuous controls. Because of the choice of  $k_* = 0$  [corresponding to  $(f_0, -f_1) \equiv (0, 0)$  in Figure 2],  $k^+(t) = k_*$  for any finite time interval can be excluded. The only piecewise continuous and constrained control which can be optimal and possibly also satisfy the maximum principle for boundary control in the distributed case is then:  $k^+(t) = k^*$  almost everywhere.

#### Properties of the Optimal Control

**Property 1:** The value of the function  $f_0$  remains constant over any finite time interval where the optimal control is unconstrained.

This property has been proven for any value of the parameter  $p$  ( $p \neq 1$ ) and  $r$  in the given problem (24) to (28). The assumption  $x_0(t) = 0$ , which was used to simplify the expressions in the lumped problem, can also be relaxed to  $x_0(t) = \text{constant}$ . The singular case where  $p = 1$  has been omitted since it was of no direct importance to the study. The property was also proven earlier for a more general class of problems with  $r = 0$  by Crowe (1972). A summary of the proof for  $r \neq 0$  and  $p \neq 1$  is given in Appendix B.

**Property 2:** The value of the hamiltonian  $H_l$  at the optimum is a strictly monotonic decreasing function of the final time  $t_f$  of the problem.

The proof of this property is by contradiction and can easily be obtained by making use of property 1 and the geometry of the velocity set and the hamiltonian lines.

This property also implies that for a fixed final time  $t_f$  the corresponding value of the hamiltonian  $H_l^+$  is unique and determines a unique Pontryagin policy. Although the Maximum Principle only gives us necessary conditions, the uniqueness of a Pontryagin policy for a problem with any fixed final time makes these conditions also sufficient in this case.

**Property 3:** There exists a critical final time  $t_{fc}$  such that for all final time  $t_f > t_{fc}$ , the optimal control policy is unconstrained for a finite time interval.

Indeed the hamiltonian line which is tangent to the velocity set for  $\phi_0$  at the extreme point  $(f_0, -f_1)$  corresponding to  $k^*$ , determines a value of  $H_{lc}^+$ , (Figure 2), which is the optimal hamiltonian value for the problem with  $t_f = t_{fc}$ . Any value of  $H_l^+ < H_{lc}^+$  corresponds to a problem with  $t_f > t_{fc}$  (Property 2). The point of support of the hamiltonian line through  $H_l^+$  with the velocity set at  $\phi_0$ , is to the left of the uppermost extreme point (Figure 2) and hence corresponds to a value of  $k^+$  which is unconstrained. Property 3 follows then from the continuity of the optimal control policy.

For the problem with the given set of parameters, the value of  $t_{fc}$  can easily be calculated and was found to be  $t_{fc} = 0.68$ . Since the maximum principle for boundary control in the distributed problem required the optimal policy to be constrained almost everywhere on the time domain, any problem with a final time which is larger than .68 constitutes a counterexample for this maximum principle.

#### NUMERICAL EXAMPLE

For the set of parameters as given in Figure 1, and a final time  $t_f = 1.0$ , the optimal control policy was indeed found to contain an unconstrained part (Figure 3). The value of  $f_0$  was found to be constant up to 5 decimals over this region at 0.82021. The optimal policy in the lumped formulation was obtained by hill-climbing on the hamiltonian  $H_l$ . This same control policy was also obtained independently, with the same accuracy, by hill-climbing on the boundary hamiltonian  $\bar{H}$  in the distributed problem.  $\bar{H}$  was found to be stationary over the unconstrained region of the optimal control policy.

The value of the objective function at the optimum was found to be  $P^+ = 0.543675$  in both the lumped and the distributed problem, whereas for the constrained policy  $k^+(t) = k^*$  we obtained  $P^* = 0.543037$ . The totally constrained policy also violated both the weak and strong maximum principles in the distributed case, in that  $\bar{H}$  had a local minimum over an initial time interval.

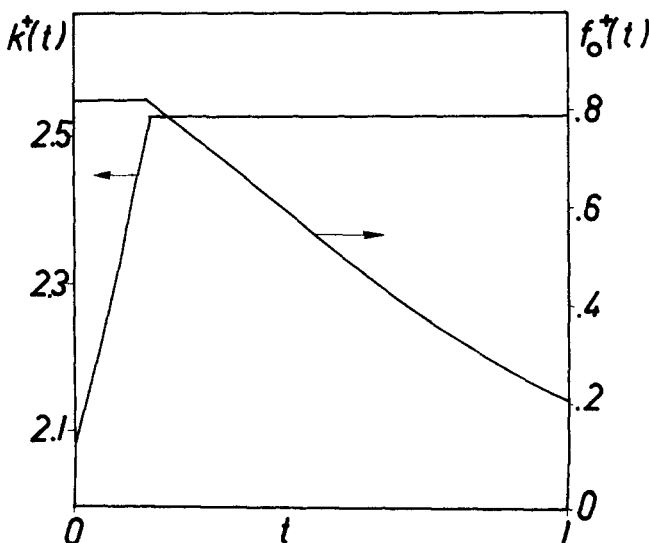


Fig. 3. Optimal control policy  $k^+(t)$  vs  $t$  and corresponding solution  $f_0(\phi^+, k^+)$  vs  $t$  for the problem with  $t_f = 1.0$ .

TABLE I. RELATIVE DIFFERENCE BETWEEN THE VALUES OF THE OBJECTIVE FUNCTION  $P_1$  AND  $P^*$  AS A FUNCTION OF  $\epsilon$

$\epsilon$	$\frac{P_1 - P^*}{P^*} \times 100$
0.150	0.510
0.125	0.579
0.100	0.660
0.075	0.751
0.050	0.856
0.030	0.953
0.020	1.005
0.010	1.061
0	1.119

For the same problem, but with  $t_f = 2.0$ , a similar control policy was found and the difference in the values of the objective function was larger:  $P^+ = 0.314603$ ;  $P^* = 0.311086$ . Fourth-order Runge-Kutta methods were used in the integration. The ordinary differential equations were integrated in 40, 80, and 100 steps and the PDE were integrated over grids of  $40 \times 40$ ,  $80 \times 80$ , and  $100 \times 100$  squares. The smallest step and grid sizes gave the best accuracy and made the results from the lumped and the distributed forms of the problem indistinguishable.

All calculations were done on a CDC 6400 computer of the McMaster Computing Centre.

#### NONORTHOGONAL CHARACTERISTICS

The problem with the skewed characteristics (17) to (18) does not lend itself to the same analysis as given above since the system of PDE cannot be lumped through a simple transformation of variables. However, it is still possible to prove that the boundary hamiltonian is strictly convex with respect to the control and therefore that the maximum principle for boundary control requires a piecewise continuous and constrained optimal policy. By choosing  $k_* = 0.0$ , we can exclude  $k^+(t) = k_*$  for any finite time interval, simply by noticing that the objective function can be increased by replacing the control over that time interval by  $k(t) = k^*$ . The only step which is missing in the analysis is the existence of an optimal controller in the class of piecewise continuous functions. It is fairly easy to show numerically that a partly unconstrained policy is superior to the best possible constrained policy  $k(t) = k^*$ .

Table I shows that for the previously used set of parameters, a final time  $t_f = 2.0$ , and decreasing values of  $\epsilon$  the relative difference in the objective functions  $P_1$  and  $P^*$  for the two policies  $k^+(t)$  and  $k^*(t)$ , respectively, remains positive and converges smoothly to the difference obtained in the orthogonal case. The partly constrained policy which was used in the calculation of  $P_1$  was the optimal policy in the orthogonal case with  $t_f = 2.0$ .

#### SUMMARY

Application of the strong maximum principle for the boundary control of a particular distributed parameter system resulted in a necessary condition which required the optimal control policy to be totally constrained.

For the limiting case of the given problem, where the characteristics became orthogonal, existence of an optimal piecewise continuous controller has been proven. It was shown that the optimal policy could be found as a unique Pontryagin policy and exhibited an unconstrained sub-policy whenever the final time was larger than a critical value.

The best constrained policy in the general case with skewed characteristics was found numerically not to be

optimal. Smoothness of the solutions was also found for a sequence of problems with skewed characteristics which converged toward the limit case with orthogonal characteristics.

We conclude that the strong maximum principle for boundary control of this class of distributed parameter systems is incorrect.

#### ACKNOWLEDGMENT

This research was supported by the National Research Council of Canada through Grant No. A953 and an NRC Scholarship. This paper is based upon one presented at the Joint Automatic Control Conference in Austin, Texas, June, 1974.

#### NOTATION

$A$	= proportionality factor between $K$ and $k^p$
$f_0, f_1$	= velocity functions, Equations (24) and (25)
$F$	= vector-valued function, Equations (1), (4)
$H$	= hamiltonian function in distributed problem
$\bar{H}$	= boundary hamiltonian function in distributed problem
$H_l$	= hamiltonian function in lumped problem
$k$	= boundary control variable, Equations (11) and (12)
$K$	= function of $k$ : $K = Ak^p$
$p$	= constant parameter in $K(k)$
$P$	= objective function
$r$	= constant parameter, Equation (12)
$S$	= unconstrained part of control policy
$t$	= dimensionless time
$u$	= boundary control, Equation (1)
$U$	= admissible control region
$v$	= state vector, Equation (1)
$\hat{V}$	= extended velocity set, Equation (29)
$x$	= state variable, Equations (11) and (12)
$z$	= dimensionless distance

#### Greek Letters

$\alpha$	= initial condition, Equation (3)
$\beta$	= boundary condition, Equation (3)
$\gamma$	= adjoint variable to $\phi$
$\lambda$	= adjoint vector, Equation (7) and adjoint variable to $x$
$\mu$	= adjoint variable to $\psi$
$\epsilon$	= small parameter, Equations (17) to (18)
$\phi$	= state variable, Equation (23)
$\psi$	= state variable, Equations (11) and (12)
$\nabla$	= gradient operator, Equation (7)

#### Subscripts

0	= initial value
c	= critical value
f	= final value
*	= minimum attainable value

#### Superscripts

+	= value along optimal policy
*	= maximum attainable value

#### LITERATURE CITED

- Bailey, J. E., "Periodic Operation of Chemical Reactors: A Review," *Chem. Eng. Communications*, 1(3), 111 (1974).  
 Butkovskii, A. G., *Distributed Control System*, pp. 38-46, Elsevier, New York (1969).  
 Chang, K. S., Ph.D. thesis, "Optimization and Optimal Control of Distributed Parameter Processes," Northwestern University, Illinois (1967).  
 ———, and S. G. Bankoff, "Optimal Control of Tubular Reactors," *AIChE J.*, 15, 410 (1969).

- Crowe, C. M., private communication (1972).
- Davis, J. M., and W. R. Perkins, "Optimal Control of Distributed Parameter Systems with Separable Controllers," *Automatica*, **8**, 187 (1972).
- Degtyarev, G. L., and T. K. Sirazetdinov, "Optimal Control of One-Dimensional Processes with Distributed Parameters," *Automation Remote Control*, **28**, 1642 (1967).
- Fjeld, M., "Relaxed Controls in Asynchronous Quenching and Dynamical Optimization," *Chem. Eng. Sci.*, **29**, 921 (1974).
- Holliday, J. H., Ph.D. thesis, "Numerical Methods for Solving Certain Distributed Parameter Optimal Control Problems," Loughborough Univ. of Technology, Leicestershire, England (1972).
- , and C. Storey, "Numerical Solution of Certain Non-Linear Distributed Parameter Optimal Control Problems," *Intern. J. Control*, **18**, 817 (1973).
- Horn, F. J., and J. E. Bailey, "An Application of the Theorem of Relaxed Control to the Problem of Increasing Catalyst Selectivity," *J. Opt. Theor. Appl.*, **2**, 441 (1968).
- Lee, E. B., and L. Markus, "Foundations of Optimal Control Theory," *The SIAM Ser. in Applied Math.*, Wiley, New York (1967).
- McShane, E. J., "Relaxed Controls and Variational Problems," *SIAM J. Control*, **5**, 438 (1967a).
- , in *Mathematical Theory of Control Processes*, A. V. Balakrishnan and L. W. Neustadt (eds.), Academic Press, New York (1967b).
- Nishida, N., A. Ichikawa, and E. Tazaki, "Optimal Design and Control in a Class of Distributed Parameter Systems Under Uncertainty," *AIChE J.*, **18**, 561 (1972).
- Ogunye, A. F., and W. H. Ray, "Optimal Control Policies for Tubular Reactors Experiencing Catalyst Decay. Part I Single Bed Reactors," *AIChE J.*, **17**, 43 (1971a).
- , "Part II Multiple-Bed Semiregenerative Reactors," *ibid.*, 365 (1971b).
- Pontryagin, L. S., V. G. Boltyanskii, R. V. Gamkrelidze and E. F. Mishchenko, *The Mathematical Theory of Optimal Processes*, Wiley, New York (1962).
- Tarasov, V. J., Ph.D. thesis, *Optimization of Multivariable Distributed Parameter Systems*, Rutgers Univ., New Brunswick, N. J. (1968).
- , H. J. Perlis, and B. Davidson, "Optimization of a Class of River Aeration Problems by the Use of Multivariable Distributed Parameter Control Theory," *Water Resources Research*, **5**, 563 (1969).
- Warga, J., "Relaxed Variational Problems," *J. Math. Anal. Appl.*, **4**, 111, 129 (1962).

## APPENDIX A. CONVEXITY OF $\bar{H}$ WITH RESPECT TO $k$

From Equations (11) and (21) follows:

$$\frac{\partial \lambda(1-x)}{\partial z} = -\mu k r(1-x)^{r-1} \quad (A.1)$$

Assuming continuity of  $x_0(t)$ ,  $k(t)$ , and  $\psi_0(z)$  guarantees the smoothness of  $\mu(z, t)$  for  $z \in [0, 1]$ ,  $t \in [0, 1]$  and from (11), (21), and (A.1) follows then:

$$\frac{\partial}{\partial z} \left( \frac{\partial \mu}{\partial t} \right) = \frac{\partial}{\partial t} \left( \frac{\partial \mu}{\partial z} \right) = \frac{\partial \mu}{\partial z} k(1-x)^{r-1} \quad (A.2)$$

For piecewise continuous control and initial conditions, the smoothness property remains valid on a finite number of subsets in the  $z \times t$  domain. Since the adjoint variables are continuous over the whole domain, the proof can be built up by the same reasoning on each subset.

From (A.2) and (22) follows:

$$\frac{\partial \mu}{\partial z} = 0 \quad \begin{array}{l} \text{for all } t \in [0, 1] \\ \text{for all } z \in [0, 1] \end{array} \quad (A.3)$$

Hence

$$\begin{aligned} \frac{\partial \mu}{\partial t} &= \frac{\partial \mu(1, t)}{\partial t} = -K(k)[1-x(1, t)] \\ &\quad + \mu(1, t)k[1-x(1, t)]^{r-1} \quad (A.4) \end{aligned}$$

and from this follows that  $\mu(z, t)$  is strictly positive for all  $t \in [0, 1]$  and zero at  $t = 1$ , unless  $x(1, t) = 1$  which requires  $x_0(t) = 1$  from (11) and may be excluded.

From (A.1) and (22) follows then also that  $\lambda$  remains strictly positive over the  $z \times t$  domain.

The second derivative of  $\bar{H}$  with respect to  $k$  is given by

$$\frac{\partial^2 \bar{H}}{\partial k^2} = \int_0^1 p(p-1)\lambda \frac{K(k)}{k^2} (1-x)\psi dz \quad (A.5)$$

and since all factors in the integrand are positive for  $p > 1$  and  $x_0(t) < 1$ , the integral will be strictly positive for all  $t \in [0, 1]$ .

## APPENDIX B. PROOF OF PROPERTY 1

Assume  $p \neq 1$  and  $r \neq 0$ .

Applying Pontryagin's maximum principle to the lumped parameter system (24) to (28), (31) and (32), with the hamiltonian  $H_l$  defined by Equation (30), leads to the following necessary conditions for optimality:

$$\frac{\partial H_l}{\partial k} = 0 \quad \text{on } S \quad (B.1)$$

where  $S$  is the unconstrained region where  $k^* < k < k^0$ ,

$$\frac{dH_l}{dt} = 0 \quad \text{for all } t \in [0, 1] \quad (B.2)$$

and

$$\frac{d}{dt} \left( \frac{k}{p-1} \frac{\partial H_l}{\partial k} \right) = 0 \quad \text{on } S \quad (B.3)$$

It is clear that all derivatives are evaluated at a Pontryagin policy.

The time derivative of Equation (27) gives

$$\frac{df_0}{dt} = \exp(-K\phi) \frac{dK\phi}{dt} \quad (B.4)$$

The derivation of the proof is then achieved in the following steps:

1. Equation (B.1) is evaluated using Equations (27), (28), and (30).

2. By using Equations (25), (28), and (31), it is possible to show that when (B.1) holds

$$\frac{d}{dt} \ln \left( \frac{k\gamma}{K} \right) = \frac{1-p}{p} \frac{d}{dt} \ln(K\phi) \quad \text{on } S \quad (B.5)$$

3. Equation (B.3) is used, together with (B.2) and (B.5) to eliminate terms involving  $\gamma$ , to yield

$$\left[ 2p-1-pK\phi + \frac{\gamma k}{K} (1-f_0)^{r-1} (pK\phi-1) \right] \frac{df_0}{dt} = 0 \quad \text{on } S \quad (B.6)$$

4. Either  $df_0/dt$  or the bracketed term equals zero. If  $df_0/dt = 0$ , the property holds. If not, the square bracket and all its time derivatives are zero. This can be used to establish that

$$\frac{d(K\phi)}{dt} = 0 \quad \text{on } S \quad (B.7)$$

which implies from (B.4) that

$$\frac{df_0}{dt} = 0 \quad \text{on } S \quad (B.8)$$

Manuscript received February 13, 1974; revision received and accepted July 17, 1974.