OPTIMIZATION BY BOUNDARY CONTROL OF REACTORS WITH DECAYING CATALYST

OPTIMIZATION BY BOUNDARY CONTROL OF REACTORS WITH DECAYING CATALYST

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DISSERTATION ABSTRACT

The quasi-steady state optimization of a single tubular fixed-bed reactor with a slowly decaying catalyst is considered.

A single irreversible reaction is considered with a rate expressible as a product of separate functions of temperature, conversion and catalyst activity. The rate of catalyst decay is also a product of separate functions of temperature, activity and conversion.

The boundary control variables are the inlet temperature, the inlet fluid flow rate and the initial catalyst activity distribution. The temperature inside the reactor is considered either uniform along the reactor axis or adiabatic. Upper and lower bounds are placed on the boundary controls. The objective function which is to be maximized measures the total amount of reaction over a fixed operating period.

Theoretical characterization of optimal control policies is obtained primarily by using a weak form of the maximum principle for boundary control.

Numerical results are presented to illustrate the optimal policies for problems where no theoretical properties were found.

The validity of a strong form of the maximum principle for boundary control of hyperbolic distributed parameter systems is critically examined.

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CHAPTER 1

INTRODUCTION

A catalytic fixed-bed tubular reactor is one of the most common types of continuous reactors used in the chemical and petrochemical process industry. One of the problems which is often encountered in these heterogeneous reaction systems is that of catalyst deactivation.

For such processes, the relative catalyst activity decreases in chronological time to such a level that it either must be regenerated or replaced by fresh catalyst.

This deactivation of the catalyst can be caused by many factors such as the influence of reactants, products and by-products, impurities in the fluid stream and the reactor operating conditions. Although the phenomenon of catalyst decay is a very complex one, it is usually possible to express the rate of decay as a simple function of catalyst activity, temperature and degree of conversion at any point inside the reactor.

Since the operating variables affect both the rate of reaction and the catalyst deactivation rate, there has been much recent interest in the optimal control of such processes.

Most work published to date has considered the optimization of reactors with both uniform and non-uniform temperature policies varying in time for which a profit function was maximized. A selection of some of the publications which led up to our present study are discussed in

Chapter 2.

In most of the previous work however, the reaction-deactivation system was described by sets of ordinary differential equations. Such systems are referred to as lumped parameter problems and the commonly used mathematical tools in the study of these optimal control problems are the classical calculus of variations and the maximum principle of Pontryagin et al. (1962).

In case the system is described by a set of simultaneous partial differential equations, the study of optimal control problems becomes much more difficult. It is only for certain forms of the system equations and for control variables which are functions of both time and position in the reactor, that a maximum principle technique, similar to Pontryagin's maximum principle, can be used.

In many physical systems however, control action can often only be taken through the natural boundaries of the space x time domain. For a catalytic reactor system for instance, such control could involve the inlet conditions into the reactor as a function of time or the composition of the catalyst bed at initial time.

For the boundary control of distributed parameter systems, several researchers have also formulated various forms of a maximum principle for optimality of the boundary control policies. Whereas for certain optimization problems a weak formulation of the maximum principle, which can also be derived from a first-order perturbation analysis of the objective function, has been stated in the literature, some authors also have stated a strong maximum principle for boundary

control of distributed parameter systems. The validity of such a strong maximum principle, which states necessary conditions for optimality similar to those of the strong maximum principle of Pontryagin and to those which have been proven for certain problems with distributed control, is critically examined in Chapter 4.

Up to date very little work has been reported for reaction-deactivation systems where the deactivation rate is dependent upon conversion. To our knowledge, no significant analytical properties of the optimal control policies have been published for such problems.

In the present study, the optimal choice of certain boundary control policies for a reaction-deactivation, where the catalyst decay is a function of conversion, has been examined. The boundary control variables which have been considered are the inlet temperature into the reactor, the inlet fluid-flow rate and the initial catalyst activity distribution along the axis of the reactor.

Basically by means of a weak maximum principle formulation for boundary control, analytical properties of the optimal control policies are derived. Numerical results are presented to illustrate features of the optimal boundary control policies of problems for which no analytical proofs were found.

In Chapter 5, we discuss in detail the problems to be considered and the quasi-steady state equations are derived.

The optimal inlet temperature policy is treated in Chapter 6 and special attention is given to the constant exit conversion property.

Chapter 7 deals with the optimal distribution of the initial

catalyst activity, both for problems with conversion independent and conversion dependent decay rates.

In Chapter 8, the simultaneous choice of the optimal inlet temperature and the optimal inlet fluid flow rate is studied.

Finally, Chapter 9 summarizes the results and conclusions obtained throughout the thesis.

CHAPTER 2

LITERATURE SURVEY

2.1 Optimal Control Theory

It is well known that for processes whose dynamic behaviour can be adequately described by a set of ordinary differential equations, the maximum principle of Pontryagin et al. (1962) can be profitably employed as a mathematical tool in optimization studies. The major advantage of using the maximum principle of Pontryagin in these lumped parameter systems is that many characteristics of the optimal control policies and optimal trajectories may be determined without solving the entire optimal control problem. Although it may not always be possible to fully characterize the optimal control policy as an explicit function of the dependent and independent variables, the results thus obtained can often be employed to reduce the dimensionality of the problem at hand and help devise simpler and more efficient algorithms to calculate a complete solution of the problem.

Examples of optimization studies, dealing with chemical reactors suffering catalyst decay, where these advantages were successfully explored can be found in the works by Ogunye and Ray (1968), Crowe (1970), Lee and Crowe (1970), and Crowe and Lee (1971).

2.1.1 Distributed Parameter Systems

A large number of optimization and optimal control problems in engineering processes, and in particular chemical processes, can adequately be described only by systems of partial differential equations. For such optimal control problems also called distributed parameter systems, the maximum principle of Pontryagin can no longer be applied.

In the last decade, a considerable amount of work has been done on the various aspects of distributed parameter control problems such as determination of necessary and sufficient conditions for optimality, observability and controllability, existence of optimal solutions and computational methods. References to these and other topics can be found in the survey papers by Butkovskii, Egorov and Lurie (1968), Robinson (1971) and Gabasov and Kirillova (1972).

Early theoretical derivations of necessary conditions were done by Butkovskii (1961a,b) for distributed systems expressed in integral equation form. An account of Butkovskii's work in this field can be found in his book (Butkovskii (1969)).

The Mayer-Bolza problem for distributed systems was formulated by Lurie (1963a,b) and necessary conditions were derived by variational techniques. Similar results were obtained by Egorov (1964, 1965a,b) for second-order hyperbolic processes and parabolic processes. A functional analysis approach was used by Katz (1964) to formulate a general maximum principle which could be applied to first-order hyperbolic, parabolic and even lumped parameter systems. In a substantial work on the theory of distributed problems, in which the concepts of controllability and observability were introduced, a general formulation of the

maximum principle was also obtained by Wang (1964). The necessary conditions obtained by Wang (1964), based on dynamic programming, are similar to those of Katz (1964).

This general approach however, has not been adopted widely in the engineering fields, mainly because of the difficulties encountered in the implementation of their general results for specific control problems.

Very recently, the functional analysis approach has regained some popularity and both analytical (Yang (1972)) and computational (Chang (1970)) efforts have been reported in the literature.

The results obtained by Katz and Wang were later also extended for the case of boundary control by Brogan (1968) but only for linear systems.

Sirazetdinov (1964), studied the optimal control of processes described by a quasilinear first-order partial differential equation with several independent variables but only one dependent variable. The necessary conditions for optimality are derived in the form of a maximum principle both for distributed controls and control variables which are a function of one independent variable only. It is also shown that this maximum principle is a sufficient condition for optimality in linear systems.

A system of two first-order partial differential equations was studied by Jackson (1966a,b). Although a more general form of the integral to be extremized was used and only an unconstrained, unbounded control vector was considered, a maximum principle formulation of

the necessary conditions was derived by variational techniques.

Volin and Ostrovskii (1964, 1965a,b) also derived necessary conditions for optimality, based on the calculus of variations, for uniform and distributed temperature control of fixed-bed tubular reactors with decaying catalyst, but no bounds were placed on the permitted temperature.

The most significant attempts to formulate a general maximum principle and which are pertinent to the formulation of a maximum principle for the type of distributed problems we will study here, are due to Chang (1967), Degtyarev and Sirazetdinov (1967) and Tarassov (1968). In these works, a maximum principle, similar to Pontryagin's maximum principle for lumped parameter systems, is formulated for distributed systems governed by a set of simultaneous first-order partial differential equations and where the control is distributed in both the time and space domains. Although these authors have used slightly different formulations of the system equations, their results are comparable since their theoretical work is an extension of the results obtained earlier by Sirazetdinov (1964). The necessary conditions are also shown to be sufficient conditions for optimality when the system consists of simultaneous linear partial differential equations.

In the case of boundary control however, there is a discrepancy in the results of these three authors. Whereas Chang and Tarassov claim a maximum principle for boundary control, similar to the one obtained for distributed control, Degtyarev and Sirazetdinov only derive necessary conditions which result in a weak maximum principle. Whereas a strong

form of the maximum principle requires a hamiltonian function to reach an absolute maximum with respect to the control at the optimum, a weak maximum principle only requires stationarity of the hamiltonian function whenever the optimal control is unconstrained and specifies a local maximum of the hamiltonian when the control is on one of its constraints. Degtyarev and Sirazetdinov further show that for the special case where both the objective function and the state equations are linear, this weak maximum principle becomes a strong one.

Ogunye and Ray (1971a,b), following Jackson's (1966) methods, also derived a generalized weak maximum principle which applies to both distributed and boundary control problems.

A great number of other workers have derived necessary conditions for systems of interest, either with theoretical analysis in mind or in order to calculate the optimal control policies numerically. Variational techniques have been used to examine problems defined either by general operators in function space or in more restricted specific forms. A selection of papers of interest are: Denn (1966), Denn, Gray and Ferron (1966), Jackson (1965, 1967), Sage and Chaudhuri (1967), Egorov (1967), Seinfeld and Lapidus (1968), Paynter (1969), Chang and Bankoff (1969), Volin et al. (1972), Holliday and Storey (1973), Johnson and Athans (1974), Bykov et al. (1973, 1974a).

2.2 Optimal Operation of Reactors with Decaying Catalyst

The optimal control of chemical reactors in which the catalyst activity decays with time has been given quite some attention in recent

years. A large number of papers have then also been published dealing with various aspects of reaction-deactivation systems. A selected review of the relevant literature up to 1970 can be found in the thesis by Therien (1971). Ray (1970) also reviewed the reported optimization work in this area up to 1970.

Therien (1971) studied the optimal distributed temperature control in a fixed-bed tubular reactor for a single irreversible reaction. Analytical properties of the optimal control policies were determined from the maximum principle formulation of Degtyarev and Sirazetdinov (1967). Results of this study have been published recently: Therien and Crowe (1974) and Crowe and Therien (1974).

The optimal control of the temperature as a function of time only for a single irreversible reaction and for both fixed and free final time problems has also been studied by Dalcorso and Bankoff (1972). The optimal temperature policy for reversible reactions with deactivation was numerically investigated by Haas et al. (1974) for an enzyme reactor in batch operation.

For optimization problems where control action is taken on the catalyst, we mention the work of Miertschin and Jackson (1970, 1971) who studied the optimal catalyst life and optimal catalyst replacement policies for both single and multiple bed tubular reactors. The problem of choosing optimal initial catalyst activity distribution profiles has also been studied by Ogunye and Ray (1971a,b) and by Nishida et al. (1972).

Although in the above mentioned works, a wide variety of reaction systems such as reversible and irreversible reactions, isothermal and

non-isothermal batch and continuous reactors, were studied both as lumped or distributed parameter systems, the catalyst decay rate expression takes on a similar form in nearly all of these studies. Following the work by Szepe (1966), the rate expression for the catalyst decay is chosen as a product of separate functions of one dependent variable only. For the most general case, these independent variables are: temperature, concentration or degree of conversion and catalyst activity. The justification of using such a decay rate expression will be dealt with in more detail in Chapter 5 of this thesis.

In most of the previous work cited however, the concentration or conversion dependent factor in the decay rate expression has been omitted. Indeed, very few results have been published to date for reaction-deactivation systems where the rate of decay is conversion-dependent.

Ajinkya and Ray (1973) used a weak form of the maximum principle to study numerically the inlet temperature control of an adiabatic axially dispersed packed bed reactor. The conversion dependency of the catalyst decay is introduced in the decay rate expression through the relationship between temperature and conversion for a single irreversible reaction in an adiabatic reactor.

A preliminary study for the optimal inlet temperature control of fixed-bed tubular reactors with decay rate expressions dependent on conversion has been done by Jutan (1973).

In a numerical study dealing with the optimal operation of fixed-bed tubular reactors where the control action consists of inducing

propagating reaction zones both concurrent and countercurrent to the fluid flow, Earp and Kerschenbaum (1975) considered in one of their problems a catalyst decay rate expression which contained a conversion dependent factor.

Bykov et al. (1973, 11974a,b), who formulated a strong maximum principle for distributed parameter systems with distributed and/or boundary control, also report some numerical results for reaction systems with conversion-dependent decay rate expressions.

Employing variational methods, Pommersheim and Chandra (1974, 1975) also calculated numerically temperature policies for batch reactors with conversion-dependent decay.

In a recent paper by Noda et al. (1975) a weak form of the maximum principle for boundary control is used to calculate optimal uniform temperature policies for a reaction deactivation system with complex reaction kinetics. Calculated results are also compared to experimental results for the dehydrogenation of isopentane where the chromia-alumina catalyst decays due to coke deposition.

Analytical results have recently been obtained by Crowe (1975) who proved the constant exit-conversion property to be optimal for a reaction-deactivation system with separable kinetics and where the decay rate is conversion dependent. These results, which are an extension of the earlier work by Szepe (1966) and Crowe (1970) have only been proven for the case of distributed temperature control.

CHAPTER 3

OPTIMAL CONTROL THEORY

3.1 Formulation of an Optimization Problem

We consider a process described by a set of simultaneous first-order partial differential equations:

$$a_i x_{it} + b_i x_{iz} = f_i(z,t,x,u) \quad i = 1,2,\ldots n \tag{3-1}$$

where x is an n dimensional state vector

$$x = \{x_1(z,t),\ x_2(z,t),\ \ldots x_n(z,t)\} \tag{3-2}$$

The subscripts t and z denote partial derivatives with respect to the independent variables t and z. The coefficients a_i and b_i, i = 1,2,...n, are considered to be real constants. The vector function $f = \{f_1, f_2, \ldots, f_n\}$ is defined on the rectangle $[t_o, t_f] \times [z_o, z_f] \equiv I \times E$ and is assumed to be at least twice continuously differentiable with respect to its arguments. The vector $u = \{u_1(z,t),\ u_2(z,t),\ \ldots, u_m(z,t)\}$ is a bounded piecewise continuous control on I x E.

In addition to (3-1), the associated initial and boundary conditions for x are given by two vector-valued functions:

$$x(z,t_o) = \alpha(z)\ ;\ x(z_o,t) = \beta(t) \tag{3-3}$$

where $\alpha_i(z)$ and $\beta_i(t)$; $i = 1,\ldots,n$, are piecewise continuous functions of z and t and have piecewise continuous first derivatives with respect to z and t along their respective boundaries of I x E. The components of the vectors $\alpha(z)$ and $\beta(t)$ can either be specified or enter the problem as boundary controls.

We introduce an objective function:

$$J = \int_{z_0}^{z_f} \int_{t_0}^{t_f} G[x(z,t),\ u(z,t)]dtdz$$

$$+ \int_{t_0}^{t_f} G_1[x(z_f,t),\ \beta(t)]dt$$

$$+ \int_{z_0}^{z_f} G_2[x(z,t_f),\ \alpha(z)]dz \qquad (3\text{-}4)$$

where G, G_1 and G_2 are twice continuously differentiable functions with respect to their arguments.

The optimization problem is then to determine u, α and β in the domain I x E such that the objective function J is maximized. The controls will be constrained by upper and lower bounds:

$$u_* \leq u \leq u^* \ ; \ \alpha_* \leq \alpha \leq \alpha^* \ ; \ \beta_* \leq \beta \leq \beta^* \qquad (3\text{-}5)$$

All controls u, α and β, satisfying the above conditions will be called admissible controls.

3.2 An Optimization Technique

We introduce the scalar Hamiltonian function H as:

$$H(z,t,x,\lambda,u) = G(x,u) + \sum_{i=1}^{n} \lambda_i(z,t)\, f_i(z,t,x,u) \tag{3-6}$$

The adjoint variables $\lambda = \{\lambda_1(z,t), \lambda_2(z,t)\ldots, \lambda_n(z,t)\}$ must be determined from the solution of the following set of equations:

$$a_i\lambda_{it} + b_i\lambda_{iz} = -\frac{\partial H}{\partial x_i} \quad i = 1,\ldots,n \tag{3-7}$$

with the associated terminal and boundary conditions:

$$a_j\lambda_j(z,t_f) = \frac{\partial G_2[x(z,t_f),\, \alpha(z)]}{\partial x_j(z,t_f)} \quad j = 1,\ldots,n \tag{3-8}$$

and

$$b_j\lambda_j(z_f,t) = \frac{\partial G_1[x(z_f,t),\, \beta(t)]}{\partial x_j(z_f,t)} \quad j = 1,\ldots,n \tag{3-9}$$

Since we will consider problems where either a_j or b_j is equal to zero, the boundary condition (3-8) or (3-9) only applies when a_j or b_j is nonzero respectively.

In a way similar to the maximum principle of Pontryagin et al. (1962), the state and adjoint equations (3-1), (3-3), (3-7)-(3-9) together with the Hamiltonian function (3-6) allow us to formulate necessary conditions for optimality.

3.3 The Maximum Principle

From the work of Degtyarev and Sirazetdinov (1967), Chang (1967), Tarassov (1968), Butkovskii (1969), Ogunye and Ray (1971a,b) and Therien (1971), we summarize the necessary conditions for optimality as they apply for our control problem (3-1)-(3-4).

3.3.1 Distributed Control

In order for an admissible control vector $u^+(z,t)$ to be optimal (i.e., to maximize J given in (3-4)) and subject to the constraints (3-1), (3-3) and (3-5), it is necessary that the Hamiltonian, defined by (3-6), reach an absolute maximum with respect to all admissible control vectors $u(z,t)$ almost everywhere in the domain I x E.

This strong form of the maximum principle can be expressed as:

$$H(z,t,x^+,\lambda^+,u^+) \geq H(z,t,x^+,\lambda^+,u) \qquad (3\text{-}10)$$

where u is an admissible control and x^+ and λ^+ are the solutions of the state and adjoint equations using the control vector u^+. The requirement that (3-10) be satisfied <u>almost everywhere</u> (a.e.) on I x E means that at any $(z,t)\epsilon I \times E$, the function H attains its maximum value except possibly on the set of $(z,t)\epsilon I \times E$ whose measure is zero.

Similar to the necessary conditions of Pontryagin's maximum principle, there is also a weak maximum principle for the distributed control problem. This weak formulation gives rise to the following necessary conditions: in order for an admissible control $u_k^+(z,t)$ $(k = 1,\ldots,m)$, to be optimal, it is necessary that

$$\frac{\partial H}{\partial u_k} = 0 \tag{3-11}$$

at u_k^+ whenever the control is unconstrained, and that H reach a local maximum with respect to the control whenever u_k^+ is on the boundary of the admissible control region given by (3-5).

3.3.2 Boundary Control

A first type of boundary control in distributed parameter systems occurs when some of the control variables u_k which appear in the state equations (3-1), are of a lower dimensionality than the state variables, i.e., $u_k(z)$ or $u_k(t)$. This type of boundary control is often referred to as "uniform control".

A weak form of the maximum principle for boundary control requires that for an admissible control $u_k^+(z)$ to be optimal, it is necessary that

$$\int_{t_o}^{t_f} \frac{\partial H}{\partial u_k} dt = 0 \tag{3-12}$$

whenever $u_k^+(z)$ is unconstrained and that $\int_{t_o}^{t_f} H dt$ reach a local maximum with respect to the control whenever the control is constrained.

The above condition needs to be satisfied almost everywhere on $[z_o, z_f] \equiv E$.

Similarly for $u_k^+(t)$ to be optimal, the conditions

$$\int_{z_o}^{z_f} \frac{\partial H}{\partial u_k} dz = 0 \tag{3-13}$$

for unconstrained $u_k^+(t)$ and $\int_{z_0}^{z_f} H dz$ reaching a local maximum whenever the control is constrained must hold almost everywhere on $[t_0,t_f] \equiv I$.

The second type of boundary control occurs when the control variables appear in the initial and boundary conditions of the state variables. For control variables of this type ($\alpha(z)$ and $\beta(t)$ in (3-3)), the necessary conditions from the weak maximum principle for boundary control become:

for the boundary control $\alpha_i^+(z)$ to be optimal, it is necessary that

$$\frac{\partial H_2}{\partial \alpha_i} \equiv 0 \tag{3-14}$$

for unconstrained α_i^+ and that

$$H_2 \equiv G_2 + \lambda_i(z,t_0)\, \alpha_i(z) \tag{3-15}$$

reach a local maximum for constrained $\alpha_i^+(z)$.

Similarly for $\beta_i^+(t)$ to be optimal, it is necessary that

$$\frac{\partial H_1}{\partial \beta_i} = 0 \tag{3-16}$$

for unconstrained β_i^+ and that

$$H_1 \equiv G_1 + \lambda_i(z_0,t)\, \beta_i(t) \tag{3-17}$$

reach a local maximum whenever $\beta_i^+(t)$ is constrained.

The weak maximum principle for boundary control leads to necessary

conditions which are similar to those derived from the weak maximum principle for distributed control. Whereas for the case of distributed control, the Hamiltonian function (3-6) is used, a boundary hamiltonian needs to be defined for the boundary control problem. For the case of "uniform control" where the control u_k is a function of z only: $u_k(z)$, a boundary hamiltonian $\overline{H}$ is defined as:

$$\overline{H} = \int_{t_o}^{t_f} H dt \tag{3-18}$$

where H is the Hamiltonian function defined by (3-6). Similarly for the case where the control is a function of t only: $u_k(t)$, the boundary hamiltonian $\overline{H}$ is given by:

$$\overline{H} = \int_{z_o}^{z_f} H dz \tag{3-19}$$

Although the formulation of a boundary hamiltonian seems rather arbitrarily chosen, Equations (3-15), (3-17), (3-18) and (3-19), it can easily be shown that the necessary conditions for optimality formulated by the weak maximum principle are identical to those obtained by considering a first-order perturbation analysis of the objective function. An illustrative example of a first-order perturbation analysis for a boundary control problem is given in Appendix B.

The term "boundary control" will be used here to describe both types of boundary control introduced above. Although we can see a distinct difference in the form of the boundary hamiltonians given by (3-15), (3-17) and (3-18), (3-19), there is no real difference between

both types of control problems. Indeed, the first type of problems, often called "uniform control" problems, merely defines a proper subset of boundary control problems of the second type.

Consider a uniform control variable $u_k(t)$ which appears in the set of state equations (3-1). By introducing a dummy state variable $x_{n+1}(z,t)$ we can eliminate $u_k(t)$ from (3-1) by replacing $u_k(t)$ with the dummy state variable wherever $u_k(t)$ appears in the state equations. The new state variable $x_{n+1}(z,t)$ can then be interpreted as the solution of the following partial differential equation:

$$\frac{\partial x_{n+1}(z,t)}{\partial z} = 0 \tag{3-20}$$

with the associated boundary condition:

$$x_{n+1}(z_o,t) = \beta_{n+1}(t) \tag{3-21}$$

With $\beta_{n+1}(t)$ identical to $u_k(t)$, the "uniform" control problem has been transformed into a boundary control problem where the control variable appears in the boundary conditions to the state equations. An analogous procedure can be used to eliminate also the uniform control variables $u_k(z)$ from the state equations.

Although such a transformation technique would allow us to deal with one type of boundary control problems only, there are two major disadvantages associated with it.

Whereas the solution of the added state equations, which determine the dummy state variables, is trivial, the additional adjoint

equations which are required for the application of the maximum principle, will in general be nonlinear and coupled with the set of n simultaneous equations given by (3-7). For the example given above with the added state equation (3-20) and after replacing $u_k(t)$ by $x_{n+1}(z,t)$ in the Hamiltonian function (3-6), the $(n+1)^{st}$ adjoint equation will take the form:

$$\frac{\partial \lambda_{n+1}(z,t)}{\partial z} = - \frac{\partial H}{\partial x_{n+1}} \tag{3-22}$$

with $\lambda_{n+1}(z_f,t) = 0$.

In case the optimal uniform control policy $u_k^+(t)$ is unconstrained over a finite time interval $(t_1,t_2) c [t_o,t_f]$, important characteristics about the optimal control on this time interval can often be determined from the necessary condition (3-13), unless the control appears linearly in the Hamiltonian function. If the first partial derivative of the boundary hamiltonian with respect to the control variable, does not contain this control variable, and vanishes over a finite time interval, the control problem is said to be <u>singular</u>. The occurrence of singular controls often leads to serious difficulties due to the fact that the application of the maximum principle loses most of its attractiveness. Because of this, many researchers have been studying the problem of singular controls and necessary conditions for optimality of such control policies have been developed. Most of this work however, was done for lumped parameter problems where the state equations are ordinary differential equations. A survey paper on singular problems in optimal control has recently been published by Bell (1975). A detailed

study on higher-order necessary conditions for optimality of controls which satisfy Pontryagin's maximum principle has been published in a three part review on singular controls by Gabasov (1971a,b,c).

For the problem described above where the uniform control variable $u_k(t)$ has been eliminated from the state equations, the boundary hamiltonian for the transformed problem becomes:

$$H_1 = G_1 + \lambda_{n+1}(z_0,t)\ \beta_{n+1}(t) \tag{3-23}$$

where $\beta_{n+1}(t)$ is the boundary control variable. Applying the necessary condition (3-16) to this problem leads to the following control characteristics:

$$\begin{aligned}
&\text{(i)} && \lambda_{n+1}(z_0,t) > 0 \Rightarrow \overset{+}{\beta}_{n+1}(t) = \overset{*}{\beta}_{n+1}(t) \\
&\text{(ii)} && \lambda_{n+1}(z_0,t) < 0 \Rightarrow \overset{+}{\beta}_{n+1}(t) = \underset{*}{\beta}_{n+1}(t) \\
&\text{(iii)} && \lambda_{n+1}(z_0,t) = 0 \Rightarrow \underset{*}{\beta}_{n+1}(t) \leq \overset{+}{\beta}_{n+1}(t) \leq \overset{*}{\beta}_{n+1}(t)
\end{aligned} \tag{3-24}$$

Optimal controls consisting of parts (i) and (ii) of (3-24) are called "bang-bang" controls. Since the control is then determined from the sign of $\lambda_{n+1}(z_0,t)$, the function $\lambda_{n+1}(z_0,t)$ is called the switching function. A total or partly singular control (iii) can exist whenever $\lambda_{n+1}(z_0,t)$ vanishes on all or part of the time domain $[t_0,t_f]$.

3.4 Existence of Optimal Control Policies

After an optimal control problem has been formulated in terms of the state equations with associated initial and boundary conditions, we are often tempted to go right ahead and use the necessary conditions of the maximum principle technique to calculate or determine properties of the optimal policies. This route of action could be a very dangerous one. The maximum principle technique provides us with the necessary conditions which will indeed be satisfied by the optimal control policy, but it gives no information about the existence of an optimal control policy. Hence it is quite feasible that for a problem which does not have an optimal solution among all possible admissible control functions, there exist one or more admissible control policies which do satisfy the necessary conditions of the maximum principle.

As practical engineers we are mostly interested in finding the optimal control policy of a problem and we hardly ever investigate the problem of existence of an optimal control in the given class of admissible control functions. Since we have formulated a "reasonable" control problem, we often believe that it is then also "reasonable" to expect that the problem has a solution. Whether or not we agree with statements as:"...it makes no sense to study a problem unless a solution can be shown to exist." or "...it makes no sense to assume the existence of a solution in a problem where there is none." (L.C. Young (1973)), the fact remains that there are problems which, although they seem to be reasonably formulated, do not permit an optimal solution in the given set of admissible control functions (see L.C. Young (1969)). An example

of an optimal control problem, where the subject of existence plays a very important role, will be treated in detail in the next chapter.

It would of course be ideal to have a set of simple rules from which existence of an optimal control for a given problem could be determined. Reality, however, is different and nearly all questions regarding existence are complicated. In studies dealing with distributed parameter systems, one often will find that none of the presently available existence theorems are suitable for a particular control problem. Moreover, since we are interested in "practical" solutions (usually piecewise continuous controls), we will frequently encounter problems where existence of an optimal control can only be proven in a class of functions which is larger than the class of piecewise continuous functions (e.g., measurable functions, relaxed or chattering controls). In order to prove existence of an optimal controller, one often needs to place the problem in a setting provided by the theory of generalized curves. A basic introduction to the concept of a "generalized curve" can be found in the book by its inventor, L.C. Young (1969). Existence theorems which make use of the theory of generalized curves for lumped parameter problems have been proven by Warga (1962; 1972); McShane (1967a,b); Lee and Markus (1967); Cesari (1965); Halkin (1965); Rubio (1975). Most of the studies done on existence deal with linear systems and very few have succeeded in developing existence theorems for optimal controls which are in the class of piecewise continuous functions (Halkin (1965)). It should also be mentioned here that when we have a problem for which existence of an optimal control has been proven in a class of functions which contain

the admissible controls as a subset, we sometimes can employ some properties of the optimal control to establish that the optimal control function is indeed a member of the admissible control set. A particular case where this technique has been successful is shown in the next chapter.

Since distributed parameter problems involve sets of partial differential equations, the development of existence theorems in this field has begun only recently. The most relevant results were first obtained by Lions (1968) and his coworkers and by Cesari (1968). Since then the field of existence studies for distributed control problems has become more and more popular and very recently a total issue of a journal has been devoted to this subject (see Cesari (1975)). The major disadvantage is the complexity of these theorems which for most of the results available to date use measure theory (Halmos (1965)) and the concept of measurable functions in their derivations (see for example, Baum (1972); Cesari and Cowles (1972)).

For all practical problems we will have to content ourselves with finding the best policy which satisfies the necessary conditions for optimality, keeping in mind that all properties derived from this will only be valid when an optimal control indeed exists in the set of admissible control functions.

3.4.1 Partial Differential Equations

One question which has not yet been discussed deals with the existence and uniqueness of a solution to the set of first-order partial differential equations defined in (3-1). In order to make certain that the optimal solution to a control problem does indeed apply to the physical system for which the state equations have been derived, the mathematical formulation itself needs to meet certain requirements. This is most commonly referred to in terms as: "The problem is well posed in the sense of Hadamard". This means that for a given set of initial and boundary conditions (3-3) and a specified vector of admissible control functions u, the set of simultaneous partial differential Equations (3-1) admits a solution for the state vector x which is unique and which depends continuously on the data for each point $(z,t) \in I \times E$. The set of state equations (3-1) is hyperbolic and is characterized by a set of n characteristic lines passing through each point (z,t) in the domain $I \times E$. When all n characteristic lines are distinct in the whole of the domain $I \times E$, the system is called totally hyperbolic. A sufficient condition now for a problem to be well posed in the sense of Hadamard is that it be totally hyperbolic (Courant and Hilbert (1962)).

Although we mainly will deal with problems which are totally hyperbolic, we will encounter some problems where not all of the characteristic directions are distinct. For these problems then we will make the assumption that they are still well posed.

CHAPTER 4

THE STRONG MAXIMUM PRINCIPLE FOR BOUNDARY CONTROL: A COUNTER EXAMPLE

4.1 The Maximum Principle for Boundary Control Problems

The strong form of the Maximum Principle of Pontryagin has been successfully extended to similar necessary conditions for optimality of distributed controls in a class of problems which are described by a set of hyperbolic partial differential equations (Degtyarev and Sirazetdinov (1967); Chang (1967); Tarassov (1968)). For the case of boundary control, where the control variable enters in the boundary conditions to the partial differential equations or where the control is a function of one variable only, Degtyarev and Sirazetdinov obtained a weaker form of the necessary conditions. Whereas the hamiltonian must reach an absolute maximum with respect to all admissible distributed controls, the boundary hamiltonian only needs to remain stationary with respect to the control in the interior of the admissible control region and must reach a local maximum when the boundary control is constrained. A similar result for the boundary control problem 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 weak maximum principle for smooth first-order distributed systems has also been found by Johnson and Athans (1974) but they did not succeed in fully developing second-order necessary conditions.

A strong form of the maximum principle for boundary control 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 controls in hyperbolic distributed parameter systems has been claimed by Chang and Bankoff (1969); Tarassov, Perlis and Davidson (1969); Lovland (1972); Holliday and Storey (1973); Bykov, et al. (1973, 1974a).

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.

For those boundary controls which appear in the state equations as functions of one independent variable only, Lovland (1972), derived a strong maximum principle for hyperbolic systems based on elementary calculus only. For boundary controls which enter in the boundary conditions of the partial differential equations, the author only derived a weak form of the maximum principle.

The strong form of the maximum principle for boundary control has also been stated by Butkovskii (1969), Nishida et al. (1972) and by Davis and Perkins (1972).

Out of all the authors mentioned above, Chang is the only one who states in his derivations of the maximum principle, both for distributed and boundary control, the requirement that the directions of the characteristics of the partial differential equations should not

coincide with those of the coordinate axes of the system. The question whether this condition is absolutely necessary for the derivation of his proofs has not been resolved as yet. From the work done by Therien (1971), we know that this condition does not have any effect on the validity of the strong maximum principle for distributed control problems. Since the proof for the boundary control problem, as given by Chang (1967), is totally based by analogy on his proof for the distributed control problem, we have reason to question the necessity of the constraints imposed on the directions of the characteristic lines. In conjunction with the formulation of a strong maximum principle for boundary control, several authors have indeed treated boundary control problems where some or all of the characteristic lines were parallel to a coordinate axis (Butkovskii (1969), Nishida et al. (1972) and Bykov et al. (1973, 1974a,b).

4.2 A Boundary Control Problem

We consider a specific problem described by

$$\epsilon_1 x_t + x_z = K(k)(1-x)\psi \tag{4-1}$$

$$\psi_t + \epsilon_2 \psi_z = - k(1-x)^r \psi \tag{4-2}$$

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

$$K = Ak^p \tag{4-3}$$

where A and p are positive parameters. The particular form of the state Equations (4-1,2) relates to the optimal inlet temperature control of a tubular fixed-bed chemical reactor with slowly decaying catalyst. It will be shown in the next chapter that Equation (4-1) represents the rate of change in conversion x for a first order irreversible reaction A → B. The temperature dependence is represented by the Arrhenius function K. The independent variable z relates to the axial distance inside the tubular reactor whereas t relates to the real time on stream.

The parameter ϵ_1 is defined as the ratio of the mean space time over the total operating time. Since ϵ_1 is very small for reactors with slowly decaying catalyst, the quasi-steady state approximation can often be used and the first term in (4-1) can be eliminated by letting $\epsilon_1 = 0$.

For $\epsilon_2 = 0$, Equation (4-2) can be recognized as a rate expression for the decay of the relative catalyst activity ψ. In order to formulate a problem where the characteristic lines do not have the same direction as one of the coordinate axes, the term with ϵ_2 has been introduced in Equation (4-2). Physically this would imply that the catalyst moves with a velocity ϵ_2 along the axis of the reactor.

Although the physical significance of the symbols used in the Equations (4-1,2) is irrelevant in the discussion of a counter-example to the strong maximum principle for boundary control, it is interesting to note that there are distributed parameter problems whose state equations are of this type.

From the problem described by the state equations (4-1,2) we will now study in detail two particular cases:

1° : $\epsilon_1 = \epsilon_2 = 0$. We will further refer to this problem as Problem $\prod_0$.

2° : $\epsilon_1 = \epsilon_2 = \epsilon > 0$. This case will be referred to as Problem $\prod_\epsilon$

4.3 Problem $\prod_0$

By letting $\epsilon_1 = \epsilon_2 = 0$ in (4-1) and (4-2), the state equations simplify to

$$x_z = K(k)(1-x)\psi \tag{4-4}$$

$$\psi_t = -k(1-x)^r\psi \tag{4-5}$$

Initial and boundary conditions to (4-4,5) are specified as

$$x(o,t) = x_o(t) \; ; \; \psi(z,o) = \psi_o(z) \tag{4-6}$$

where $x_o(t)$ and $\psi_o(z)$ are piecewise continuous functions and

$$0 \leq x_o(t) \leq 1 \; ; \; 0 < \psi_o(z) < \infty \tag{4-7}$$

The admissible control region is defined as

$$U = \{k | k_* \leq k(t) \leq k^*\} \tag{4-8}$$

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 by

$$P = \int_0^1 [x(1,t) - x_0(t)]dt \tag{4-9}$$

4.3.1 Application of the Maximum Principle for Boundary Control

For the boundary control problem (4-4) - (4-9), we define a hamiltonian function H as

$$H = \lambda\, K(k)(1-x)\psi - \mu\, k(1-x)^r\psi \tag{4-10}$$

where the adjoint variables $\lambda(z,t)$ and $\mu(z,t)$ are given by:

$$\lambda_z = -\frac{\partial H}{\partial x} = \lambda\, K(k)\psi - \mu\, kr(1-x)^{r-1}\psi \tag{4-11}$$

$$\mu_t = -\frac{\partial H}{\partial \psi} = -\lambda\, K(k)(1-x) + \mu\, k(1-x)^r \tag{4-12}$$

with terminal and boundary conditions

$$\lambda(1,t) = 1 \; ; \; \mu(z,1) = 0 \tag{4-13}$$

The boundary hamiltonian $\overline{H}$ is defined as in (3-19) by

$$\overline{H} = \int_0^1 H dz \tag{4-14}$$

It is possible to prove analytically (Appendix C) that for all

values of the parameter p greater than 1, the boundary hamiltonian $\bar{H}$ is a strictly convex function of k. Hence since $\bar{H}$ is a continuous function of k, $\bar{H}$ can only attain 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 $t \in [o,1]$.

4.3.2 Equivalent Lumped Parameter System

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

$$\phi(t) = \int_o^1 \psi(z,t)dz \tag{4-15}$$

and letting $x_o(t) = 0$ for convenience, the problem (4-4) - (4-9) can be written as

$$\max_{k(t)\in U} P = \max_{k(t)\in U} \int_o^1 f(\phi,k)dt \tag{4-16}$$

$$\frac{d\phi}{dt} = g(\phi,k) \tag{4-17}$$

with the initial condition

$$\phi(o) = \phi_o = \int_o^1 \psi_o(z)dz \tag{4-18}$$

The functions f and g in (4-16) and (4-17) will be called the "velocities"

and are given by

$$f(\phi,k) = 1 - \exp(-K(k)\phi) \tag{4-19}$$

$$g(\phi,k) = \frac{-k}{rK(k)} (1 - \exp(-rK(k)\phi)) \tag{4-20}$$

Equations (4-19) and (4-20) are obtained by substituting the explicit solution for x from (4-4) into (4-5) and integrating (4-5) over the z-domain.

In order to deal with the subject of existence of an optimal controller, we introduce the concept of the extended velocity set as used by Lee and Markus (1967). For our problem (4-16)(4-17), the extended velocity set $\hat{V}(\phi)$ is defined as

$$\hat{V}(\phi) = \{f(\phi,k),\ g(\phi,k) | k_* \leq k \leq k^*\} \tag{4-21}$$

The set of parameters which will be used in the further development has been chosen as

$$\begin{aligned} p &= 1.5 \\ r &= 0.2 \\ k_* &= 0.0 \\ k^* &= 2.5265 \\ A &= .573364 \\ \phi_0 &= 1.0 \end{aligned} \tag{4-22}$$

For the given set of parameters the extended velocity set $\hat{V}(\phi)$ has been calculated for various values of ϕ and a graph representing the

points (f, -g) is shown in Figure 4-1. For a given value of ϕ, the velocity line has a sigmoid shape but loses its inflection point as ϕ decreases. The point (o,o) in Figure 4-1 corresponds to $k = k_*$ whereas point A corresponds to $k = k^*$ for $\phi = 1$.

4.3.3 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), Young (1969), Bailey (1974), Fjeld (1974)).

Whereas a classical control policy $k(t) \in U$ allows us to reach any point (f,g) in the velocity set $\hat{V}(\phi)$, the main importance of a relaxed controller in our problem is that the set of reachability can be extended to all points (f,g) in the convex hull of the set $\hat{V}(\phi)$.

Since $\hat{V}(\phi)$ in our problem consists of two velocity function, we need two classical admissible control functions $k_1(t)$ and $k_2(t)$ in order to obtain a relaxed controller. Suppose that for $\phi = 1$ the points of the extended velocity set which correspond to the values of k_1 and k_2 are given by (f_1,g_1) and (f_2,g_2). As illustrated in Figure 4-2, any point on the line connecting $(f_1,-g_1)$ and $(f_2,-g_2)$ in the graph for $\phi = 1$, can then be reached by using a relaxed control which is the limit of very fast switching between $k_1(t)$ and $k_2(t)$. In a mathematical formulation this means that for relaxed controllers the functions f and g in

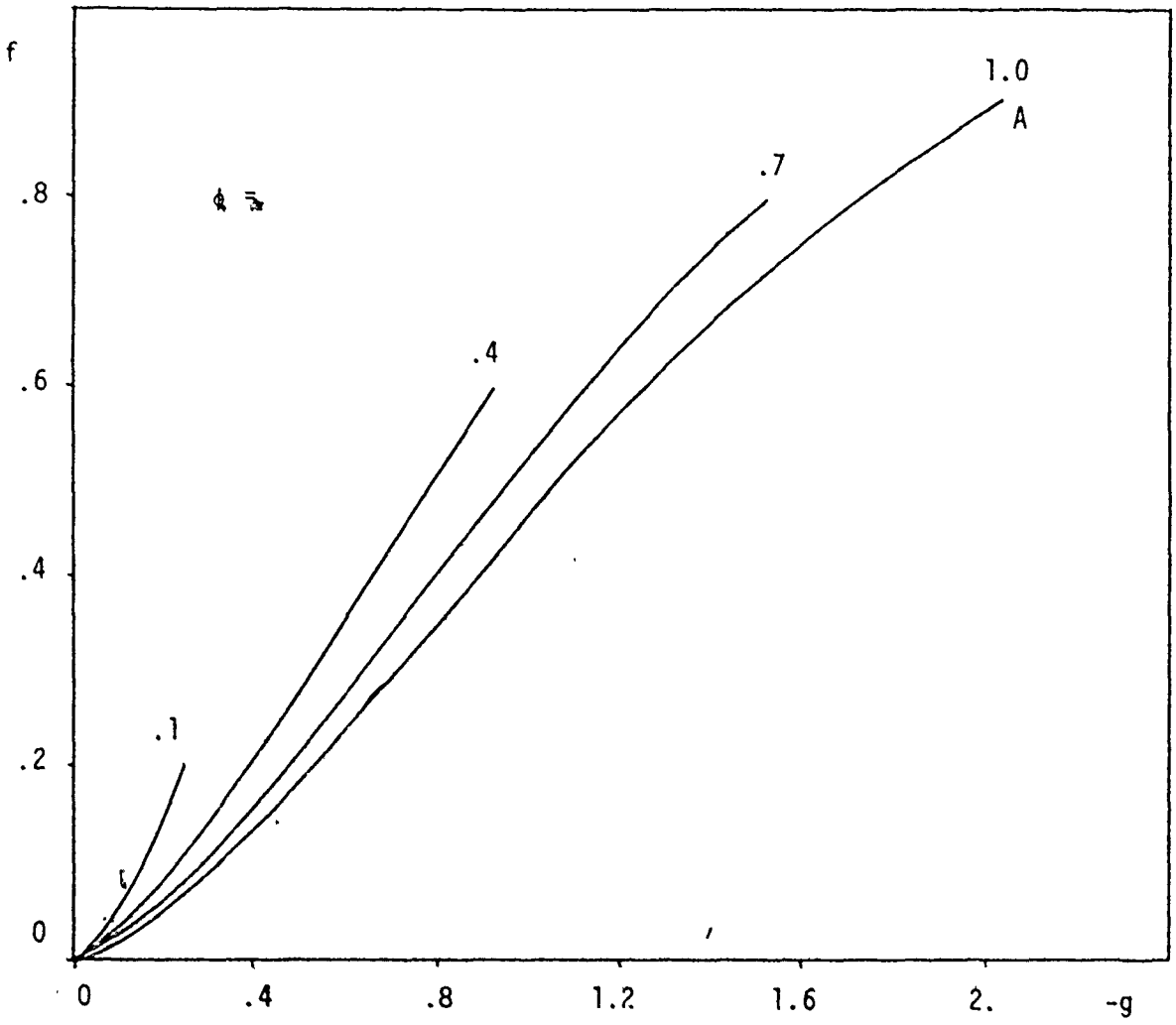

Figure 4-1: Graph of the extended velocity set $\hat{V}(\phi)$ plotted as f vs. - g.

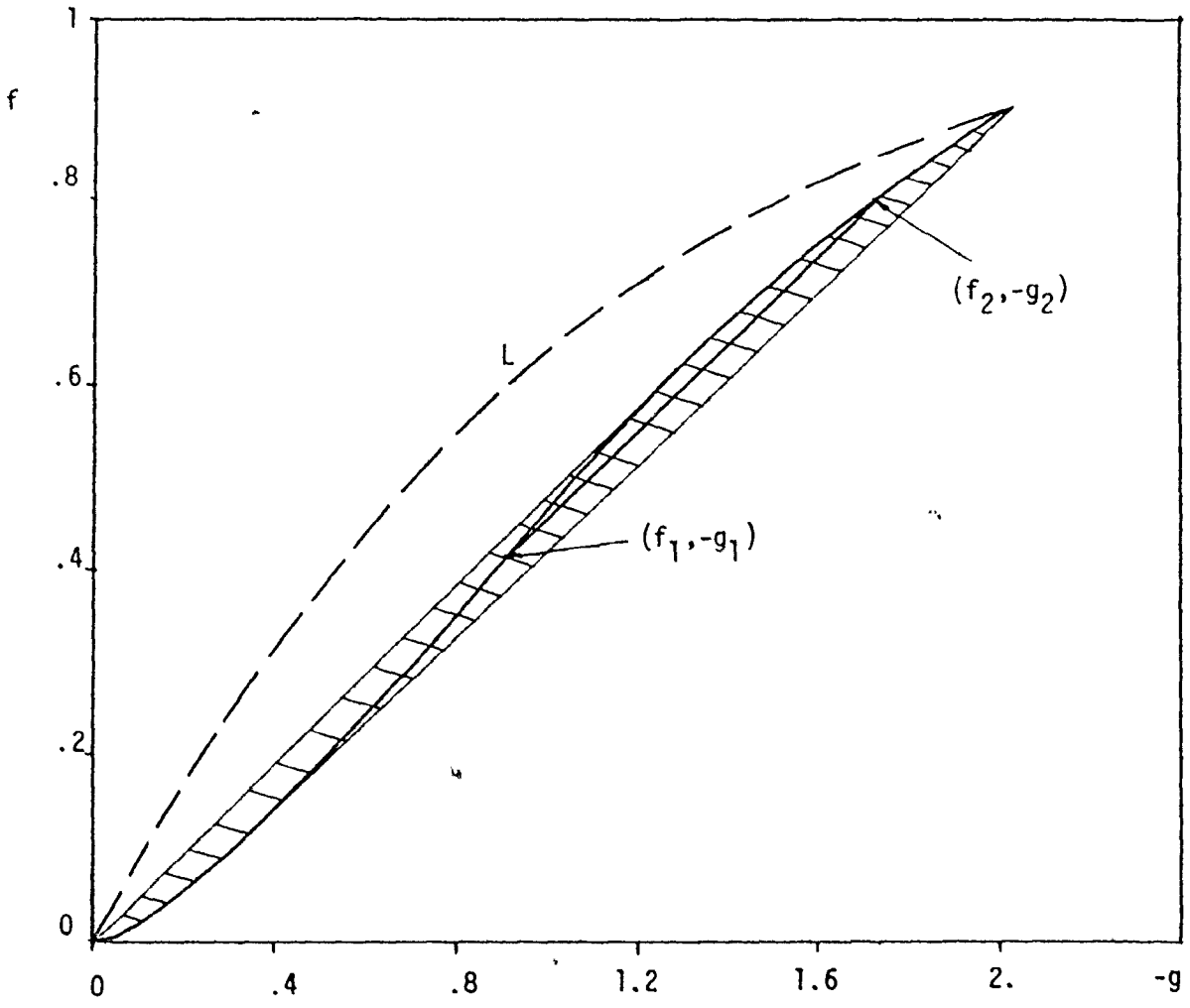

Figure 4-2: Graphs of the convex hull of $\hat{V}(\phi)\big|_{\phi=1}$ and the set L of endpoints $(f(\phi,k^*), g(\phi,k^*) | 0 \leq \phi \leq 1)$.

(4-16) and (4-17) can be replaced by

$$\bar{f}(\phi,\bar{k}) = \alpha(t)\, f(\phi,k_1) + (1 - \alpha(t))\, f(\phi,k_2) \tag{4-23}$$

$$\bar{g}(\phi,\bar{k}) = \alpha(t)\, g(\phi,k_1) + (1 - \alpha(t))\, g(\phi,k_2) \tag{4-24}$$

respectively with $0 \leq \alpha(t) \leq 1$. The functions $\alpha(t)$, $k_1(t)$ and $k_2(t)$ are then all parts of the relaxed control policy $\bar{k}(t)$. Since for $k_1(t)$ and $k_2(t)$ we can choose any admissible regular control policy, all points of the convex hull of $\hat{V}(\phi)$ are reachable by a relaxed controller.

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 $(f,g) \in \hat{V}(\phi)$ as classical controllers and those corresponding to points $(\bar{f},\bar{g}) \in co\hat{V}(\phi)$ but $\notin \hat{V}(\phi)$ as pure relaxed controllers. If $k_1(t) = k_2(t) = k(t)$, the relaxed controller $\bar{k}(t)$ is identical to the classical controller $k(t)$ and $\bar{f}$ and $\bar{g}$ can be replaced by f and g.

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

4.3.4 Application of Pontryagin's Maximum Principle

A hamiltonian function H_ℓ for the lumped parameter system (4-16) to (4-20) is defined as

$$H_\ell = \bar{f} + \gamma\bar{g} \tag{4-25}$$

with the adjoint variable γ given by

$$\frac{d\gamma}{dt} = -\frac{\partial H_\ell}{\partial \phi} \tag{4-26}$$

and

$$\gamma(1) = 0 \tag{4-27}$$

An optimal relaxed control policy $\bar{k}^+(t)$ then satisfies the maximum principle for lumped parameter systems (Pontryagin et al. (1962), McShane (1967b)) and the corresponding value of the hamiltonian H_ℓ^+ remains constant almost everywhere on the time domain. Using (4-27), H_ℓ^+ is given by

$$H_\ell^+ = H_\ell^+\Big|_{t=1} = \bar{f}(\phi(1), \bar{k}^+(1)) \tag{4-28}$$

Since f is a strictly monotonic increasing function of k, the maximum principle requires that $\bar{k}^+(1) = k^*$. Equation (4-28) can then be rewritten as

$$H_\ell^+ = f(\phi(1), k^*) \tag{4-29}$$

and since $\phi(1) > 0$ for all problems with finite final time, H_ℓ^+ is strictly positive.

By rearranging (4-25) as follows:

$$\bar{f} = H_\ell + \gamma(-\bar{g}) \tag{4-30}$$

the value of the hamiltonian H_ℓ is given in the graph $\bar{f}$ vs. $(-\bar{g})$ in Figure 4-3 by the intercept of the f axis with a hamiltonian line going through a point $(\bar{f},-\bar{g})$ with slope γ. For an optimal control policy, it is

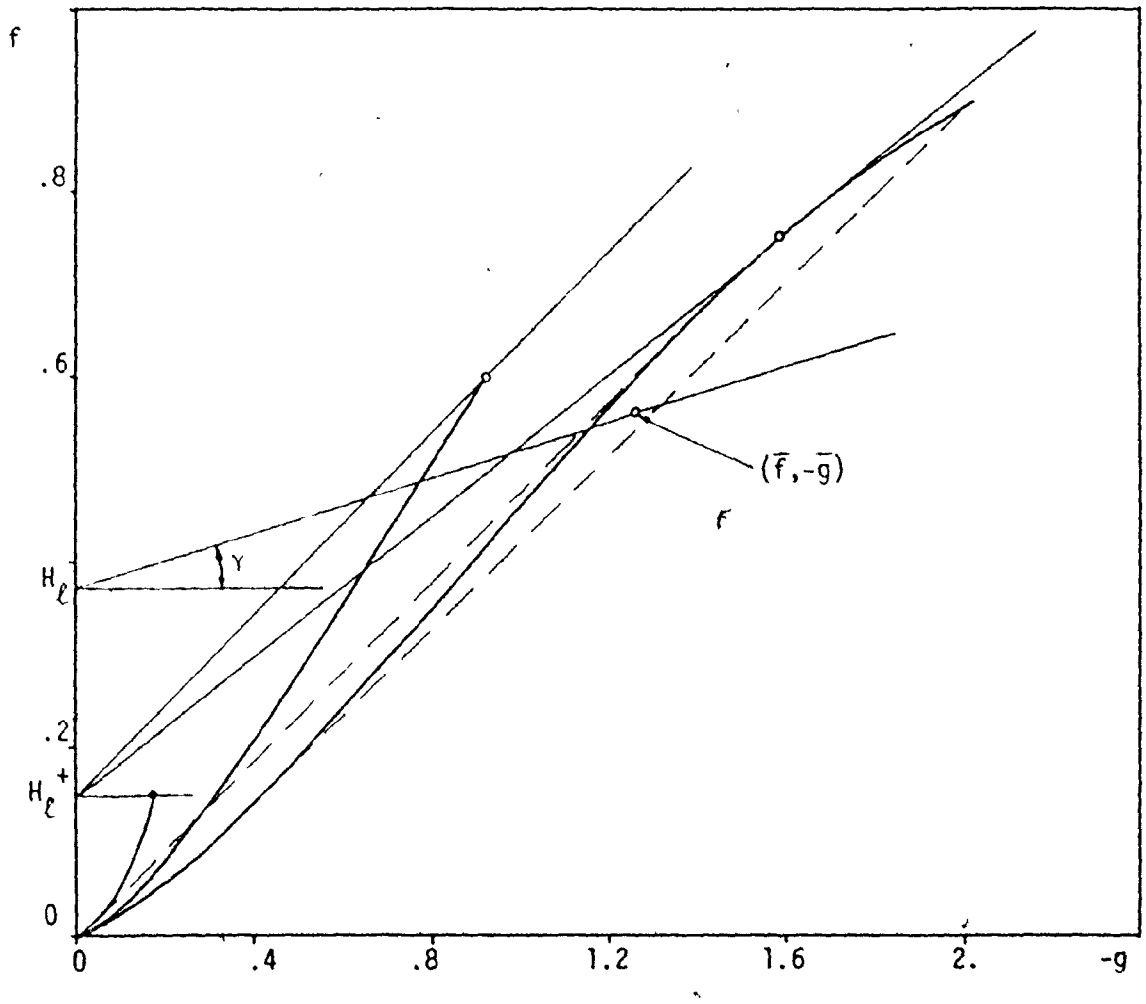

Figure 4-3: Graph of $\hat{V}(\phi)$ and hamiltonian lines $\bar{f} = H_\ell + \gamma(-\bar{g})$.

necessary, in order to maximize H_ℓ, that for any given value of ϕ, the point (or points) of support $(\bar{f},-\bar{g})$ in the graph which are lying on the hamiltonian line, correspond either to the uppermost extreme point (where $k = k^*$) and/or the point (or points) of tangency of a hamiltonian line with slope γ, which is tangent from above to the set of points $(\bar{f},-\bar{g})$ in the graph. Furthermore, all hamiltonian lines, corresponding to different values of ϕ, have the point H_ℓ^+ on the f axis in common for the optimal control policy $\bar{k}^+(t)$ (Figure 4-3).

Since $H_\ell^+ > 0$ and through the geometry of the set of points $(\bar{f},-\bar{g})$ in the graph, the point of support $(\bar{f},-\bar{g})$ at the optimum and for any given value of ϕ is unique and belongs to the graph of points corresponding to the velocity set $\hat{V}(\phi)$ itself. The corresponding optimal controller is therefore a classical controller. Since both f and g are continuous functions of ϕ and k, for $k(t)\in U$, the optimal controller $k^+(t)$ will also be a continuous function and hence belongs to the class of piecewise continuous controllers.

4.3.5 Properties of the Optimal Control

Property 1: An admissible control policy $k(t)$ which consists of $k(t) = k_*$ over a finite time interval cannot be optimal.

Proof:

Since $\gamma(t)$ is the solution of the ordinary differential equation (4-26) with terminal condition (4-27), $\gamma(t)$ is continuous, non-negative and finite for all $t \in [o,1]$. Because of the choice of $k_* = 0$ (corresponding to $(f,-g) \equiv (o,o)$ in Figure 4-3), the value of the hamiltonian H_ℓ

becomes zero whenever $k(t) = k_*$. Since $H_\ell^+ > 0$, $k(t) = k_*$ for a finite time interval cannot form part of the optimal control policy $k^+(t)$.

Property 2: The value of the function f remains constant over any finite time interval where the optimal control is unconstrained.

This property has been proven for any value of the parameters $p(p \neq 1)$ and r in the given problem (4-16) to (4-20). The assumption $x_0(t) = 0$, which was used in 4.3.2 to simplify the expressions in the lumped parameter problem, can also be relaxed to $x_0(t) =$ constant. The singular case where $p = 1$ has been omitted since it is of no direct importance in this study. This property has also been proven earlier for a more general class of problems with $r = 0$ by Crowe (1970). The proof of Property 2 for $r \neq 0$ and $p \neq 1$ is given in Appendix D.

Property 3: 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.

Proof:

Let $H_1^+(H_2^+)$ denote the value of the hamiltonian H_ℓ at the optimum for the problem with final time $t_{f1}(t_{f2})$ and let $H_1^+ > H_2^+$ (Figure 4-4).

A. Assume $t_{f1} \geq t_{f2}$. (4-31)

Since $H_1^+ > H_2^+$, any optimal hamiltonian line originating from H_1^+ has a point of support $(f_1^+, -g_1^+)$ which is to the right of the point of support $(f_2^+, -g_2^+)$ whenever $k_2^+(t) < k^*$ and coincides with $(f_2^+, -g_2^+)$

when $k_2^+(t) = k^*$ (Figure 4-4). This implies that

$$g_1^+ \leq g_2^+ \tag{4-32}$$

for all $t \in [o, t_{f2}]$. From (4-17),(4-31) and the fact that $g^+ < 0$ (since $k^+(t) > 0$ for any problem with finite final time) (4-32) implies

$$\phi(t_{f1}) \leq \phi(t_{f2}) \tag{4-33}$$

From $H_1^+ > H_2^+$, $\gamma(t_f) = 0$ and the geometry of the graph of the extended velocity set $\hat{V}(\phi)$ it follows that

$$\phi(t_{f1}) > \phi(t_{f2}) \tag{4-34}$$

(see Figure 4-4 and Figure 4-1). Hence a contradiction which means that (4-31) is impossible and we get

$$H_1^+ > H_2^+ \Longrightarrow t_{f1} < t_{f2} \tag{4-35}$$

B. Using identical arguments it is easy to establish that

$$t_{f1} < t_{f2} \Longrightarrow H_1^+ > H_2^+ \tag{4-36}$$

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 $k^+(t)$. Although the Maximum Principle only provides us with necessary conditions, the uniqueness of a Pontryagin policy for a problem with any fixed final time makes these conditions also sufficient ones.

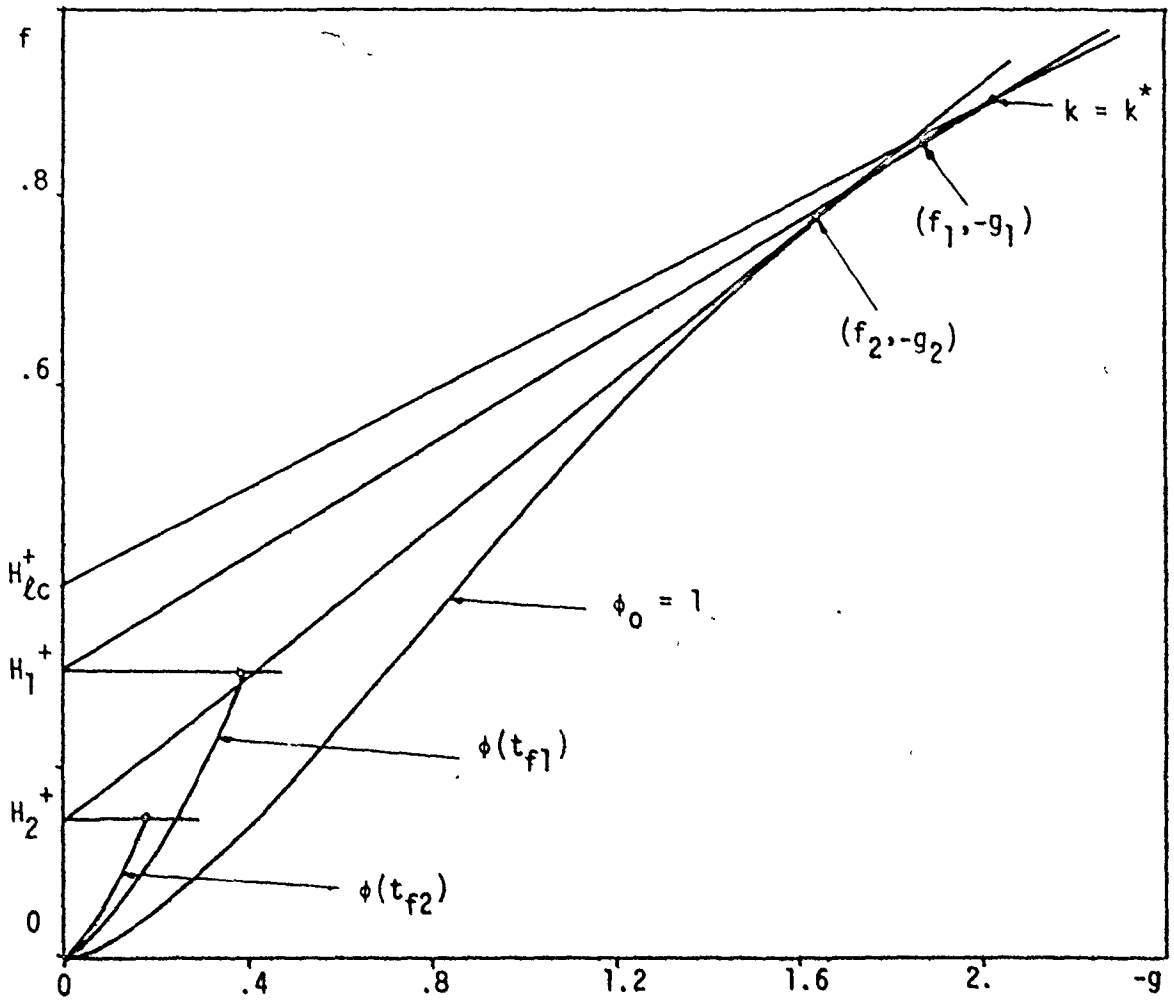

Figure 4-4: Hamiltonian lines at the optimum for problems with different final times.

Property 4: There exists a critical final time t_{fc} such that for any problem with a final time $t_f > t_{fc}$, the optimal control policy is unconstrained for a finite time interval.

Proof:

The hamiltonian line which is tangent to the graph of the velocity set for ϕ_o at the extreme point (f,-g) corresponding to k^*, determines a value of $H_{\ell c}^+$, (Figure 4-4), which is the optimal hamiltonian value for the problem with $t_f = t_{fc}$. Any value of $H_\ell^+ < H_{\ell c}^+$ corresponds to a problem with $t_f > t_{fc}$ (Property 3). The point of support of the optimal hamiltonian line through H_ℓ^+ with the velocity set at ϕ_o is then to the left of the uppermost extreme point and hence corresponds to a value of $k^+ < k^*$. Property 4 follows then from the continuity of $k^+(t)$.

For our problem with the given set of parameters (4-22) and $\phi_o = 1$, the value of t_{fc} can easily be calculated and was found to be $t_{fc} = 0.68$. Since from 4.3.1, the maximum principle for boundary control required the optimal control policy for Problem $\boxed{\ }_o$ to be constrained almost everywhere on the time domain $[o,t_f]$, any such problem with a final time t_f which is larger than t_{fc} constitutes a counter example for this maximum principle.

4.3.6 Numerical Results

The optimal policy $k^+(t)$ for Problem $\boxed{\ }_o$ with the set of parameters given by (4-22) and a final time $t_f = 1.0$ was indeed found to contain an unconstrained part over a finite time interval (Figure 4-5).

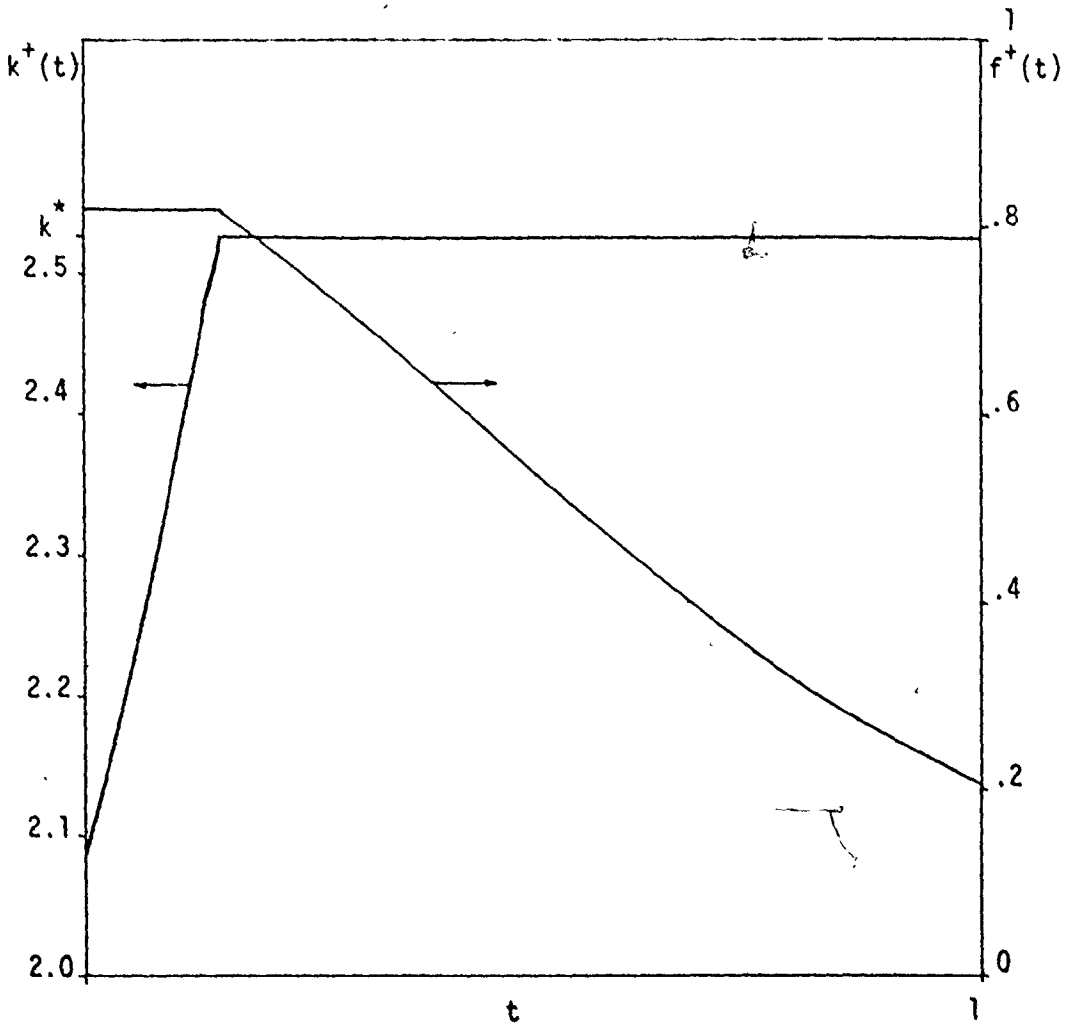

Figure 4-5: Optimal control $k^+(t)$ and $f^+(t)$ for Problem Π_0 with $t_f = 1$.

The value of f^+ was also found to remain constant up to 5 decimals accuracy ($f^+ = 0.82021$) over the region where the control is unconstrained. The value of the objective function at the optimum was calculated as $P^+ = 0.543675$ whereas for the best totally constrained policy $k(t) = k^*$ for all $t \in [0,1]$, we obtained $P^* = 0.543037$. The optimal policy was first calculated from the lumped formulation of the problem by hill-climbing on the hamiltonian H_ℓ using the following procedure:

1°: Choose a control policy $k_0(t)$.

2°: Integrate the state equation (4-17) forwards over the time domain.

3°: Evaluate f (4-13) and the value of the objective function P (4-16).

4°: Integrate the adjoint equation (4-26) backwards over the time domain.

5°: Using the calculated solutions for the state and adjoint variables, evaluate the hamiltonian H_ℓ and the derivative $\partial H_\ell / \partial k$.

6°: Calculate

$$k_i(t) = k_{i-1}(t) + \eta \frac{\partial H_\ell}{\partial k} \qquad i = 1,2,.... \qquad (4\text{-}37)$$

where η is a positive parameter. Set $k_i(t) = k^*(k_*)$ whenever (4-37) results in $k_i(t) > k^*(< k_*)$. Return to point 2°. This iterative procedure can be halted when either the increment in the value of the

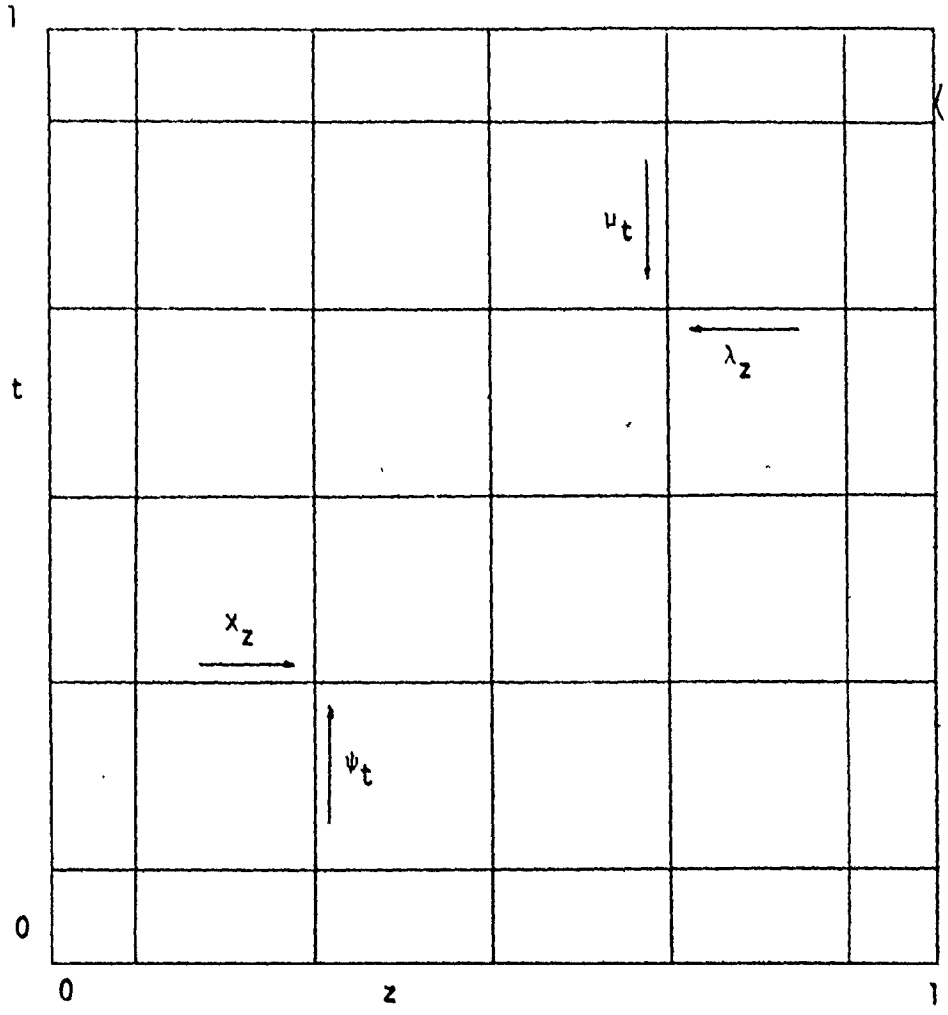

Figure 4-6: Characteristic lines for Problem Π_0.

objective function becomes very small or the new policy $k_i(t)$ is sufficiently close to the previous one $k_{i-1}(t)$. A third-order Runge-Kutta method was used in the integration of the ordinary differential equations. The value of the objective function P was calculated from (4-16) by using the trapezium-rule. The time domain [o,1] was divided into 40, 80 and 100 equal intervals and the accuracy of the results increased with the number of intervals.

At the optimum, the value of the hamiltonian was constant up to 5 decimals ($H_\ell^+ = .20914$) and the first derivative of H_ℓ with respect to k over the unconstrained region was of the order 10^{-9} to 10^{-10}. The calculated policy $k^+(t)$ corresponded to a maximum of the hamiltonian H_ℓ since the second derivative of H_ℓ with respect to k was negative and varied from -.25 to -.17 over the unconstrained region.

The same control policy $k^+(t)$ was also obtained independently, with the same accuracy, by hill-climbing on the boundary hamiltonian $\bar{H}$ in the distributed version of the problem. For the integration of the partial differential Equations (4-4), (4-5), (4-11) and (4-12), we make use of the method of characteristics. Since the characteristic lines s_1 and s_2 for Problem Π_0 are orthogonal and parallel to the coordinate axes (Figure 4-6), the state and adjoint equations can be integrated as ordinary differential equations in the z and t directions. The calculations are done in a sequence similar to the procedure described above, for the lumped case. Since the state and the adjoint equations are coupled, an iterative technique has to be used in order to calculate the state and adjoint variables at each grid point. The z x t domain

Table 4-1: Calculated values of the objective function in the lumped and the distributed case for the optimal policy $k^+(t)$ and the constrained policy $k(t) = k^*$. The parameter n equals the number of intervals in which the time domain was divided in the lumped case and the grid size (n x n) in the distributed case.

n	Policy	Lumped System	Distributed System
40	$k^+(t)$	.5436726	.5436696
	k^*	.5430358	.5430361
80	$k^+(t)$	.5436749	.5436743
	k^*	.5430371	.5430373
100	$k^+(t)$	.5436751	.5436748
	k^*	.5430371	.5430374

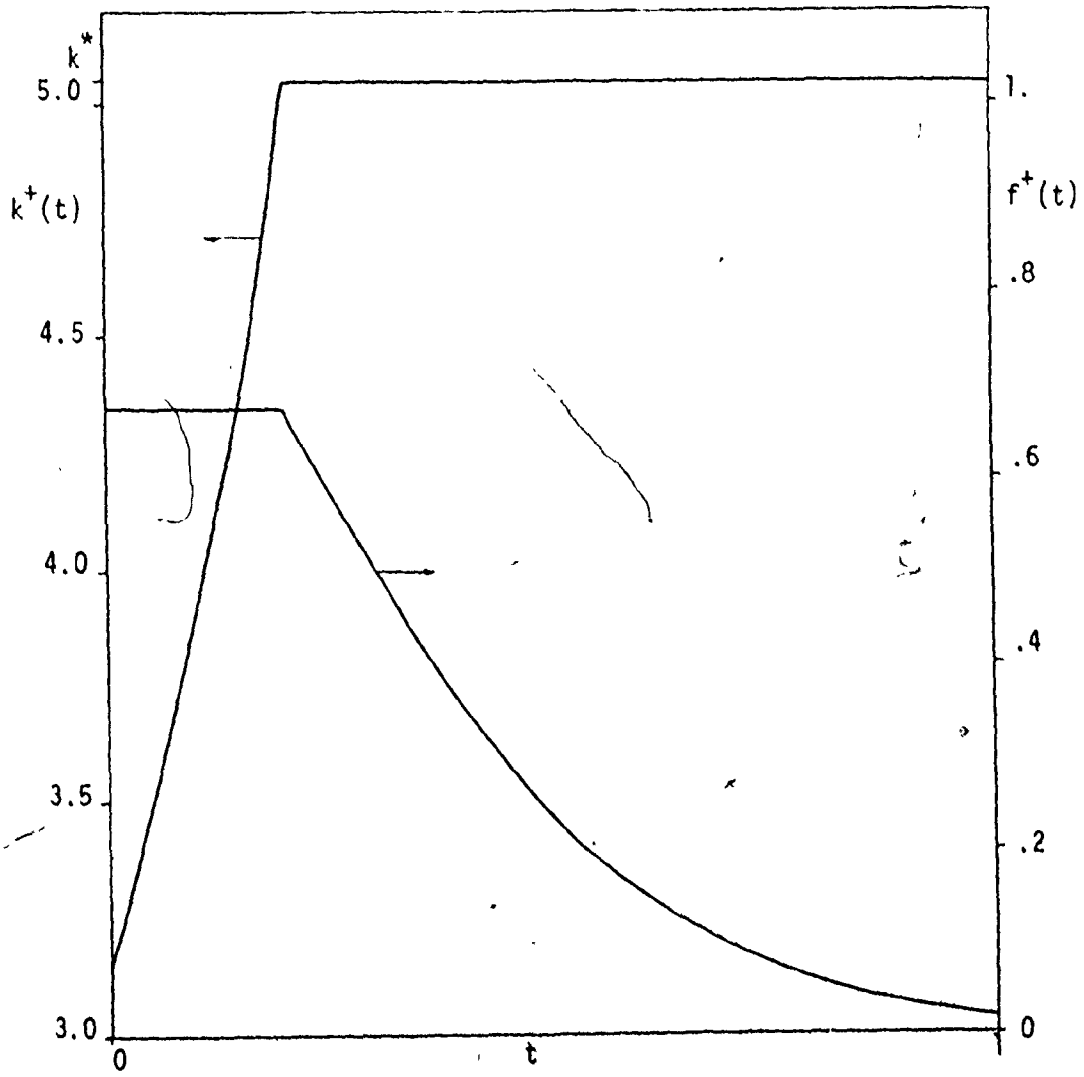

Figure 4-7: Optimal control $k^+(t)$ and $f^+(t)$ for Problem Π_0 with $t_f = 2.$

was divided into grids of 40 x 40 , 80 x 80 and 100 x 100 equal squares. The accuracy of the results again increased with the number of grids. For the smallest grid size (100 x 100), the calculated values of $x^+(1,t)$ were indistinguishable from those of $f^+(t)$ in the lumped case.

For the optimal policy $k^+(t)$, the boundary hamiltonian $\bar{H}$ remained constant (up to 5 decimals accuracy) over the unconstrained region ($\bar{H}^+ = -.20371$) and the first derivative of $\bar{H}$ with respect to k was of the order of 10^{-5}. The boundary hamiltonian however, reached a minimum at $k^+(t)$ and the value of the second derivative ranged from .07 to .05 over the unconstrained region.

The best totally constrained policy $k(t) = k^*$ for all $t \in [o,1]$ also violated the strong maximum principle for boundary control in that $\partial\bar{H}/\partial k$ was definitely negative for a finite time interval. For instance at $t = 0$, $\partial\bar{H}/\partial k$ was equal to -.05 for the totally constrained policy and was 1.10^{-5} for the optimal policy $k^+(t)$.

Table 4-1 gives a summary of the calculated values of the objective function for both the lumped and the distributed case with the various number of intervals used in the integration.

For the same problem, but with the final time $t_f = 2.0$, a similar optimal control policy was found (Figure 4-7) and the difference in the values of the objective function was larger: $P^+ = 0.3146026$; $P^* = 0.3110862$.

4.3.7 Pseudo Relaxed Control

In the discussion under 4.3.3, we have seen that by introducing relaxed controllers in the lumped parameter problem, the velocity functions f and g can be replaced by "effective velocities". These "effective velocity functions" are defined as a convex combination of velocities which can be reached by classical controllers.

The concept of a relaxed controller can now be extended to distributed parameter problems both for distributed and boundary controls. Restricting ourselves to the study of boundary control problems, a relaxed boundary control can again be defined as the limit of very fast switching between two or more admissible classical boundary control policies. For the boundary control problem with state equations (4-1) and (4-2), we can define the right hand sides of these partial differential equations as "velocities". For a relaxed boundary control, these velocity functions can then be replaced by "effective velocities". For example, the state equations (4-1), (4-2) for a relaxed boundary control become:

$$\varepsilon_1 x_t + x_z = \alpha(t)K(k_1)(1-x)\psi + (1-\alpha(t))K(k_2)(1-x)\psi \qquad (4\text{-}38)$$

$$\psi_t + \varepsilon_2\psi_z = -[\alpha(t)k_1(1-x)^r\psi + (1-\alpha(t))k_2(1-x)^r\psi] \qquad (4\text{-}39)$$

where $k_1(t)$ and $k_2(t)$ are admissible boundary controls and $\alpha(t)$ is a piecewise continuous function of t with $0 \leq \alpha(t) \leq 1$.

Since K(k) and k appear linearly in the state equations (4-1)-(4-2), we can rearrange (4-38) and (4-39) as follows:

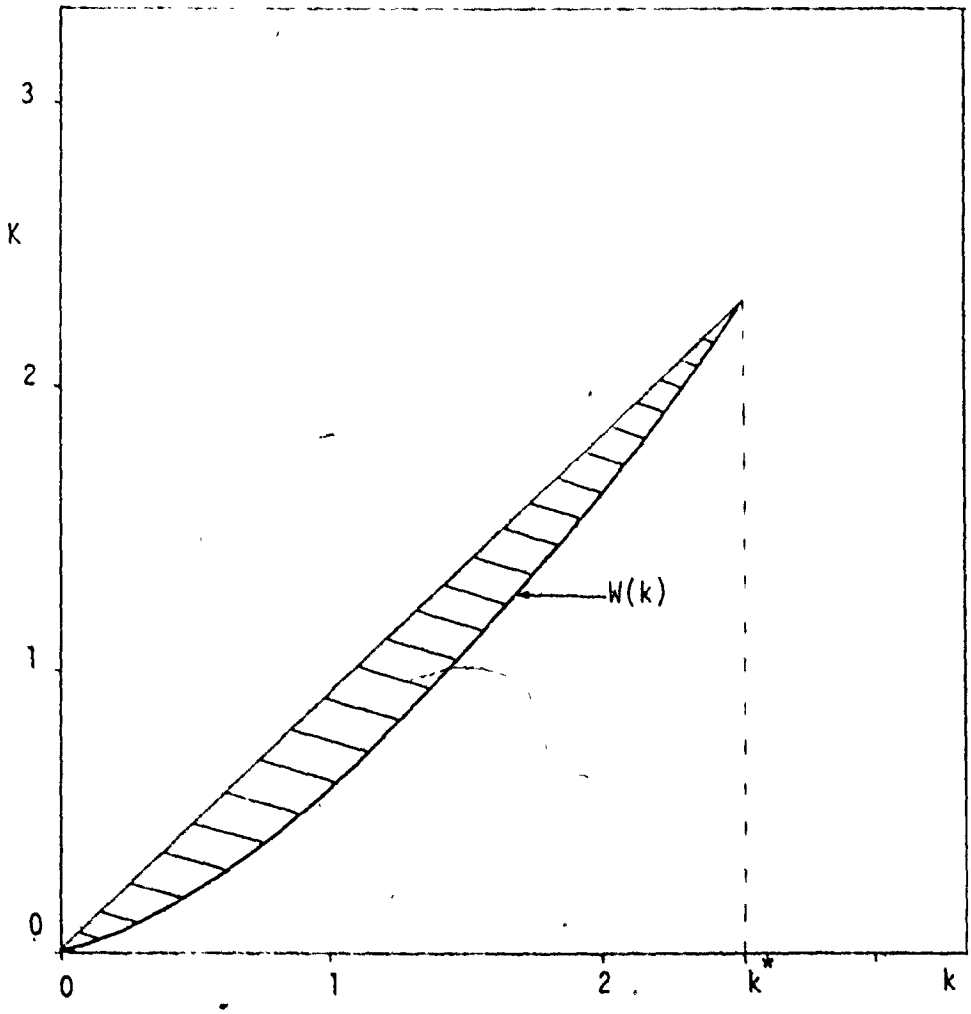

Figure 4-8: Graph of the control set W(k) and co W(k) with parameters given by Equation (4-22).

$$e_1 x_t + x_z = (\alpha(t)K(k_1) + (1-\alpha(t))K(k_2))(1-x)\psi \tag{4-40}$$

$$\psi_t + e_2\psi_z = -(\alpha(t)k_1 + (1-\alpha(t))k_2)(1-x)^r\psi \tag{4-41}$$

The relaxed control can be denoted by $(\bar{K},\bar{k})$ where

$$\bar{K} = \alpha(t)K(k_1) + (1-\alpha(t))K(k_2) \tag{4-42}$$

$$\bar{k} = \alpha(t)k_1 + (1-\alpha(t))k_2 \tag{4-43}$$

By defining the control set W(k) as

$$W(k) = \{K(k),k \mid k_* \leq k \leq k^*\} \tag{4-44}$$

it follows from (4-42) and (4-43) that any relaxed control $(\bar{K},\bar{k})$ belongs to the convex hull of W(k), (Figure 4-8).

Since the state equations of Problem Π_0 (4-4) and (4-5) are derived from (4-1) and (4-2) by letting $e_1 = e_2 = 0$, it would seem reasonable, at least at first sight, to define a relaxed boundary controller for Problem Π_0. However, as we will show, this relaxed boundary control for Problem Π_0 is not feasible.

Let us first consider the state equation (4-5). Since the characteristic lines s_2 for this partial differential equation are parallel to the t-axis (Figure 4-6), the rate of change of ψ along the t-direction is identical to the rate of change of ψ along the characteristic direction s_2. (Note that this is not the case for the general equation (4-2) when $e_2 \neq 0$). We will refer to the right-hand side expression of (4-5) as the "velocity of ψ along t". Let $k_1(t)$ and $k_2(t)$ be two admissible classical boundary control functions which are defined over a finite

open time interval (t_1,t_2) c[o,1]. A particular relaxed boundary control can then be constructed on (t_1,t_2) in the following manner:

1°: Divide the open interval (t_1,t_2) into an even number of equal open sub-intervals Δt_i, i = 1,2,....n.

2°: Define a control function $k_o(t)$ as

$$k_o(t) = \begin{cases} k_1(t) \text{ on } \Delta t_i \text{ for all odd values of } i < n \\ \\ k_2(t) \text{ on } \Delta t_i \text{ for all even values of } i \leq n \end{cases}$$

Over the time interval (t_1,t_2), the control $k_o(t)$ is at $k_1(t)(k_2(t))$ for a finite time interval Δt_i and then switches instantaneously to the other control $k_2(t)(k_1(t))$. Accordingly the velocity of ψ along t is characterized by the same number of switches between $-k_1(1-x)^r\psi$ and $-k_2(1-x)^r\psi$ on (t_1,t_2). We now repeat the procedure 1° and 2° for each open time interval Δt_i, i = 1,2,....n. By repeating this for each newly created set of open time intervals, a sequence of control functions $k_o(t)$ is obtained. The number of switches between $k_1(t)$ and $k_2(t)$ increases and the time spent on either control level before a switch occurs, decreases as the sequence of controls $k_o(t)$ is formed. Similarly the velocity of ψ along t switches back and forth between the two velocity levels at an ever increasing rate. In the limit, the frequency of switching becomes infinite and the sequence of controls $k_o(t)$ converges to a relaxed boundary control $\bar{k}(t)$ as defined by (4-43). The value of

the function $\alpha(t)$ depends on the way the intervals were divided in step 1° and on the type of definition given for $k_0(t)$ in step 2°. The velocity of ψ along t then also switches infinitely fast between $-k_1(1-x)^r\psi$ and $-k_2(1-x)^r\psi$ over the open time interval (t_1,t_2). Hence the effective velocity of ψ along t becomes $-\bar{k}(1-x)^r\psi$ over that time interval.

The influence of a relaxed controller on the velocity term in Equation (4-4) is different however. Indeed, since the characteristic lines s_1 for this partial differential equation are parallel to the z-axis, the right-hand side of (4-4) expresses the velocity of x along z. This means that the frequency of switching in the sequence of controls $k_0(t)$ does not have any effect on this velocity term since the value of the control remains constant over the whole z-domain [o,1]. For the general Equation (4-1) with $e_1 \neq 0$, the velocity term includes a rate of change of x in the t-direction and switching of this velocity term would occur since the characteristic lines for this state equation would indeed be cut by the lines along which the control is discontinuous. A relaxed controller which results in effective velocity functions as given in (4-40) and (4-41) is therefore not feasible in Problem $\prod_0$.

Nevertheless, we will investigate the influence of a relaxed boundary controller on the performance index P in Problem $\prod_0$ anyway. Although this might seem to be absurd, the importance of this will become relevant in the discussion of the relaxed controllers for Problem $\prod_e$ which will be dealt with below. Since for Problem $\prod_0$, the relaxed controller is not realizable, we will call it a <u>pseudo-relaxed controller</u>.

Since the boundary hamiltonian for Problem Π_0 is a strictly convex function of k, we will consider a pseudo-relaxed control which chatters between the upper and lower constraints k^* and k_*. With $k_* = 0.0$, the pseudo-relaxed control (4-42) (4-43) can be written as $\bar{K} = \alpha(t)K(k^*)$; $\bar{k} = \alpha(t)k^*$. Substituting these into the equations for the lumped parameter system (4-16) to (4-20) gives

$$f(\alpha\phi, k^*) = 1 - \exp(-\alpha K(k^*)\phi) \tag{4-45}$$

$$g(\alpha\phi, k^*) = \frac{-k^*}{r\,K(k^*)}(1 - \exp(-r\,\alpha\,K(k^*)\phi) \tag{4-46}$$

where $\alpha(t)$ is now the control variable with $0 \leq \alpha(t) \leq 1$. The velocity set V_R defined as

$$V_R(\phi) = \{f(\alpha\phi, k^*),\ g(\alpha\phi, k^*) \mid 0 \leq \alpha \leq 1\} \tag{4-47}$$

is then for all values of $\phi (0 \leq \phi \leq 1)$, a subset of the set L of end-points corresponding to $k = k^*$ of the extended velocity set $\hat{V}(\phi)$ given by (4-21). As illustrated in Figure (4-2) for $\phi = 1 (V_R(\phi)|_{\phi=1} \equiv L)$, the pseudo-relaxed controllers are infeasible since the only points of the graph of $V_R(\phi)$ which are contained in the graph of the convex hull of $\hat{V}(\phi)$ are those corresponding to $\alpha = 0$ and $\alpha = 1$.

Applying Pontryagin's maximum principle to the pseudo-relaxed control problem, assuming that an optimal pseudo-relaxed control policy exists, allows us to establish the following property of the optimal policy $\alpha^+(t)$.

$\alpha^+(t)\,\phi^+(t)$ = constant on any finite time interval

(t_1, t_2) c[0,1] where $0 < \alpha^+(t) < 1$. $(r \neq 1)$.

Proof:

From the expression of the hamiltonian H_ℓ

$$H_\ell = (1 - \exp(-\alpha K(k^*)\phi) - \frac{\gamma k^*}{r K(k^*)} (1 - \exp(-r \alpha K(k^*)\phi) \quad (4\text{-}48)$$

with

$$\frac{d\gamma}{dt} = -\alpha K(k^*) \exp(-\alpha K(k^*)\phi) + \gamma k^* \alpha \exp(-r \alpha K(k^*)\phi) \quad (4\text{-}49)$$

and $\gamma(1) = 0$, we obtain

$$\frac{\partial H}{\partial \alpha} = K(k^*)\phi \exp(-\alpha K(k^*)\phi) - \gamma k^* \phi \exp(-r \alpha K(k^*)\phi) = 0 \quad (4\text{-}50)$$

on (t_1, t_2).

Making use of (4-49) and (4-50), we also get

$$\frac{d}{dt}\left(\frac{\partial H}{\partial \alpha}\right) = (r-1)(K(k^*))^2 \phi \exp(-\alpha K(k^*)\phi) \frac{d\,\alpha\,\phi}{dt} = 0 \quad (4\text{-}51)$$

on (t_1, t_2). Hence it follows that for $r \neq 1$ the product $\alpha\phi$ = constant at the optimum. Q.E.D.

From the definition of f in (4-45) we also have that the value of f remains constant over the time interval where the optimal control policy $\alpha^+(t)$ is unconstrained.

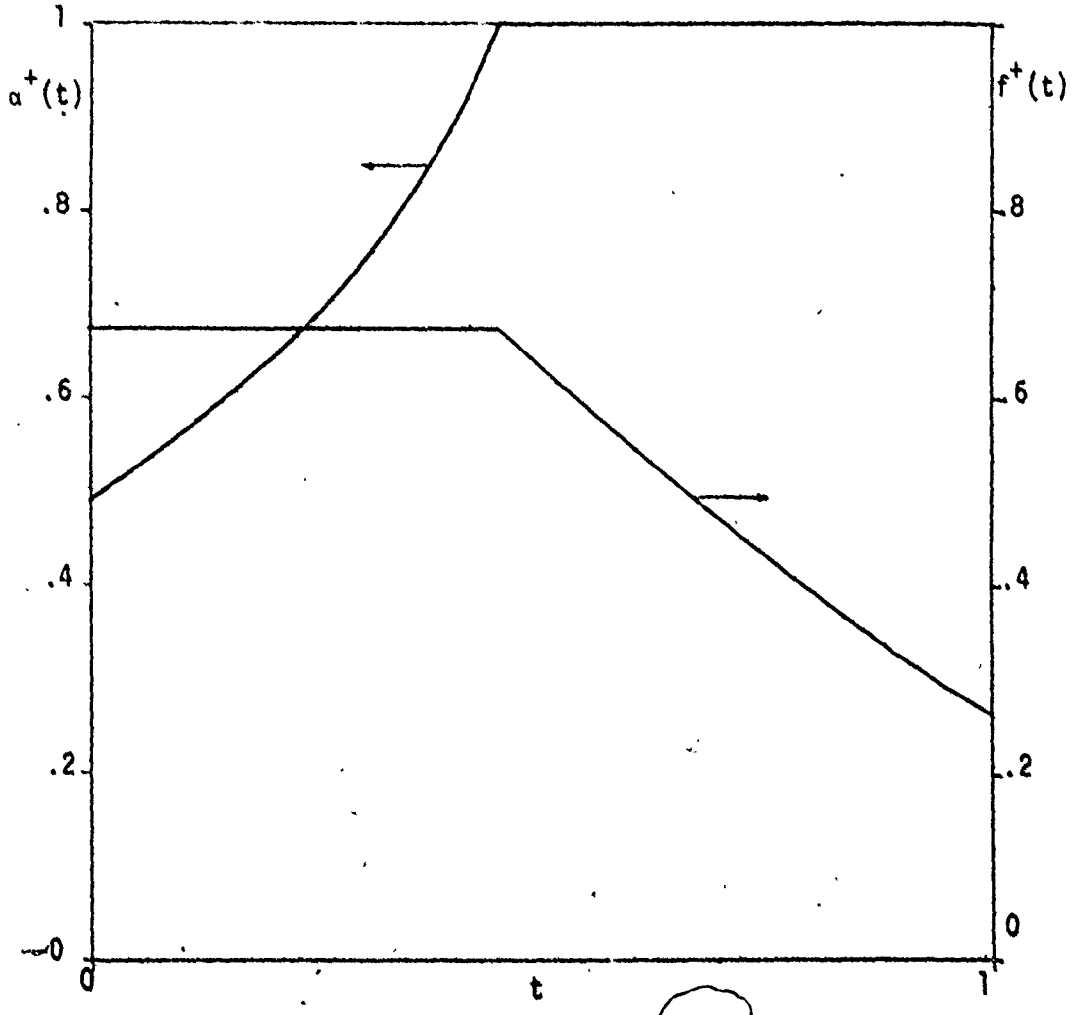

Figure 4-9: Optimal pseudo-relaxed control policy $a^+(t)$ and corresponding $f^+(t)$ for problem Γ_0.

The optimal policy $\alpha^+(t)$ has been calculated for the pseudo-relaxed problem with the same parameters (4-22) and with $\phi_o = 1.0$, $t_f = 1.0$ (Figure 4-9). The corresponding value of the objective function P_R^+ was found to be considerably larger than the optimum for Problem Π_o: $P_R^+ = .5593447$ compared to $P^+ = .5436751$ from Table 4-1.

4.4 Problem Π_e

For the problem with state equations

$$\epsilon x_t + x_z = K(k)(1-x)\psi \tag{4-52}$$

$$\psi_t + \epsilon\psi_z = -k(1-x)^r\psi \tag{4-53}$$

the characteristic lines s_1 and s_2 are straight lines in the z x t domain which for small values of ϵ form angles of the order of ϵ radians with respect to the coordinate axes (Figure 4-10). We assume $\epsilon < 0$. The set of ordinary differential equations which describes the system along the characteristic lines are then

$$\frac{dx}{ds_1} = K(k)(1-x)\psi \tag{4-54}$$

$$\frac{d\psi}{ds_2} = -k(1-x)^r\psi \tag{4-55}$$

and appear to be identical to those for Problem Π_o. The major difference however is that the control k does not remain constant along the characteristic lines s_1, since they are no longer parallel to the z-axis.

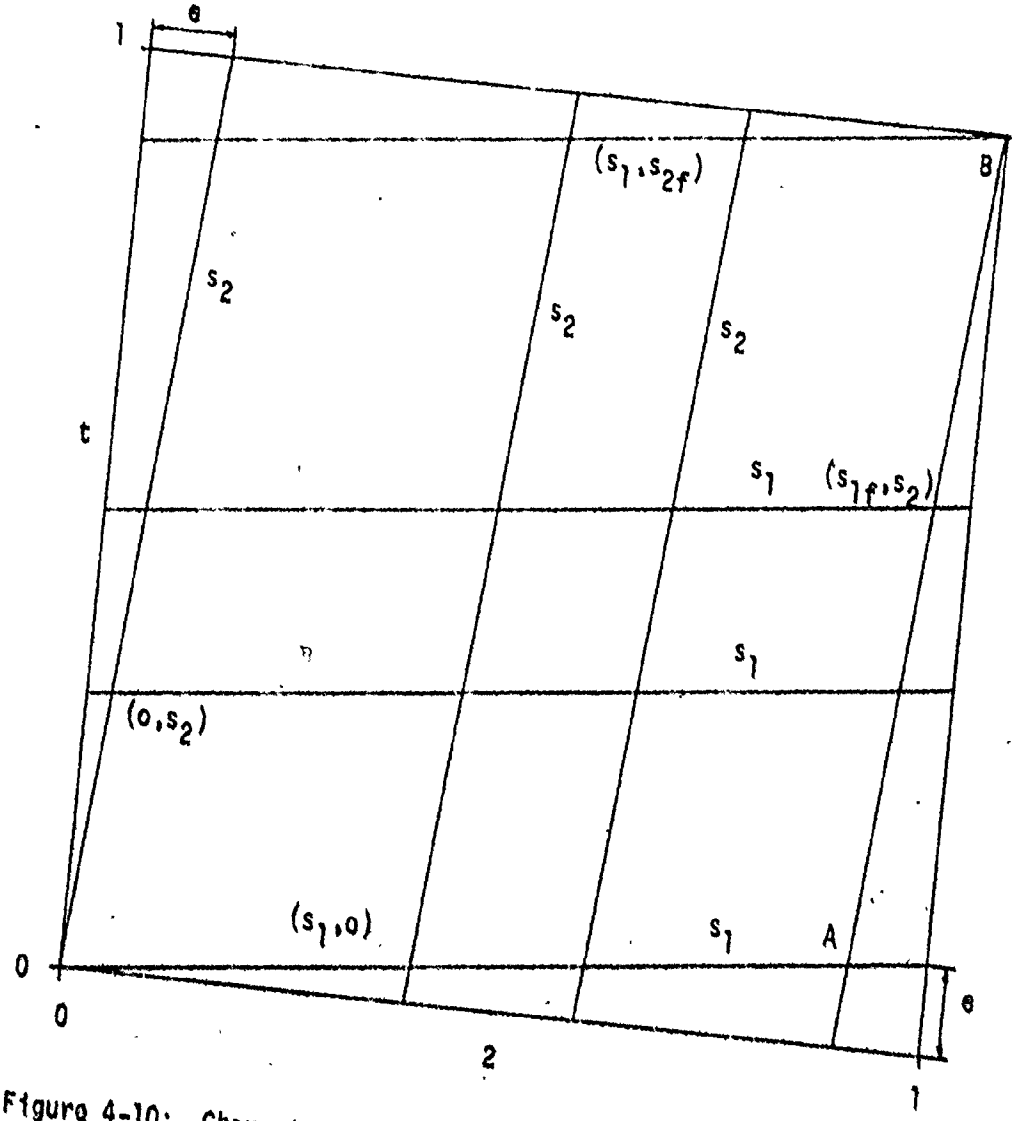

Figure 4-10: Characteristic lines s_1 and s_2 for Problem Γ_0.

As a result of this, Problem $\prod_e$ cannot be transformed into a lumped parameter problem and the existence of an optimal boundary control in the class of piecewise continuous functions cannot be established by lumping the problem.

In order to simplify the computational algorithms and the theoretical analysis in the study of this problem, the initial and boundary conditions to (4-52) and (4-53) are defined as:

$$x(o,t) = \begin{cases} x_o(t) & \text{for } t \in [o,1-e] \\ 1 & \text{for } t \in (1-e,1] \end{cases}$$

$$x(z,o) = 1 \qquad \text{for } z \in [o,1] \tag{4-56}$$

$$\psi(o,t) = 0 \qquad \text{for } t \in [o,1]$$

$$\psi(z,o) = \begin{cases} \psi_o(z) & \text{for } z \in [o,1-e] \\ 0 & \text{for } z \in (1-e,1] \end{cases}$$

where $x_o(t)$ and $\psi_o(z)$ are piecewise continuous functions and

$$0 \leq x_o(t) \leq 1 \; ; \; o < \psi_o(z) < \infty \tag{4-57}$$

Since any discontinuity in the state variables is carried through along the characteristic lines, the advantage of this choice of initial and boundary conditions is that the only region of interest in the whole z x t domain is enclosed by the characteristic lines s_1 and s_2 going through the

points (o,o) and (1,1). This domain of interest will be denoted as the $s_1 \times s_2$ domain where s_1 varies from 0 to s_{1f} and s_2 varies from 0 to s_{2f} (Figure 4-10). In the remainder of the whole z x t domain, the right-hand side expressions of (4-52) and (4-53) are identically zero. The initial and boundary conditions which have been specified along the co-ordinate axes can therefore be carried over without change along their appropriate characteristic directions to form the initial and boundary conditions for the $s_1 \times s_2$ domain.

The admissible control region is again defined as

$$U = \{k \mid k_* \leq k(t) \leq k^*\} \tag{4-58}$$

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 by

$$P = \int_0^1 [x(1,t) - x(o,t)]dt \tag{4-59}$$

4.4.1 Application of the Maximum Principle for Boundary Control

The boundary hamiltonian for Problem Π_2 is defined as

$$H = \int_0^1 H dz \tag{4-60}$$

where

$$H = \lambda K(k)(1-x)\psi - \mu k(1-x)^n\psi \tag{4-61}$$

Although some authors use different formulations for the hamiltonian function (Chang (1967), Tarassov (1968), Butkovskii (1969), Lovland (1972)), the definition of the hamiltonian as given in (4-61) is equivalent to the other forms with the exception of terms which are not explicit functions of the control.

The adjoint equations are

$$\theta\,\lambda_t + \lambda_z = \lambda\,K(k)\psi - \mu k r(1-x)^{r-1}\psi \tag{4-62}$$

$$\mu_t + \theta\,\mu_z = -\lambda\,K(k)(1-x) + \mu k(1-x)^r \tag{4-63}$$

with terminal and boundary conditions

$$\begin{aligned} &\lambda(1,t) = 1\ ;\ \lambda(z,1) = 0 \\ &\mu(1,t) = 0\ ;\ \mu(z,1) = 0 \end{aligned} \tag{4-64}$$

Since the characteristic lines for (4-62), (4-63) coincide with those for the state equations (4-52), (4-53), the adjoint equations can also be written as

$$\frac{d\lambda}{ds_1} = \lambda\,K(k)\psi - \mu k r(1-x)^{r-1}\psi \tag{4-65}$$

$$\frac{d\mu}{ds_2} = -\lambda\,K(k)(1-x) + \mu k(1-x)^r \tag{4-66}$$

Because of the definition of the initial and boundary conditions (4-56), the adjoint variables λ and μ do not undergo any change outside the s_1 x s_2 domain and hence the terminal and boundary conditions (4-64) can be

carried along their appropriate characteristic lines to form terminal and boundary conditions to (4-65) and (4-66) of the $s_1 \times s_2$ domain. Since the $s_1 \times s_2$ domain is the only region of interest, it is also more convenient to formulate the objective function P between the initial and final points A and B of the characteristic line s_2 at s_{1f} (Figure 4-10):

$$P = \int_A^B [x(s_{1f}, s_2) - x_0(s_2)] ds_2 \tag{4-67}$$

We must realize of course that in the $s_1 \times s_2$ domain, the boundary control k(t) becomes a function of both s_1 and s_2 since the lines along which k remains constant are no longer parallel to the s_1 characteristics. Any given policy $k(s_1, s_2)$ needs then also to be specified along the two boundary lines of the $s_1 \times s_2$ domain where $s_1 = 0$ and $s_2 = s_{2f}$ respectively. Whereas the hamiltonian function (4-61) remains unchanged, the boundary hamiltonian $\bar{H}$ needs to be evaluated as the integral of H along the lines where the control remains constant.

As was the case for Problem Π_0, it is still possible to prove analytically that, for the case $p > 1$, $\bar{H}$ is a strictly convex function of the boundary control k (Appendix E). In case an optimal piecewise continuous control exists for Problem Π_a, the strong maximum principle then again requires the optimal control to be totally constrained almost everywhere.

4.4.2 Numerical Results

For the integration of the state and adjoint equations, a grid, formed by intersecting characteristic lines s_1 and s_2, is constructed in the $s_1 \times s_2$ domain. Since for a given boundary control policy, the control $k(s_1,s_2)$ can be calculated at each point of the grid, the integration of the Equations (4-54), (4-55), (4-65), and (4-66) can be carried out in the same way as in Problem Π_0.

For different values of e, the value of the objective function P^* corresponding to the totally constrained control k^* was compared to the value of P obtained from an arbitrarily chosen partly unconstrained control k(t). The set of parameters used was the same as for Problem Π_0 with $x_0(t) = 0$, $\psi_0(z) = 1$ and $t_f = 2.0$. The partly unconstrained policy k(t) was chosen as the optimal policy $k^+(t)$ for the same problem with $e = 0$. The results are tabulated in Table 4-2.

From the values of P^* and P in Table 4-2 follows:

1°: The totally constrained policy k^* is not optimal since there exists at least one partly unconstrained policy for which the objective function is larger than P^*.

2°: For a given admissible control policy and decreasing values of e, the value of the objective function converges smoothly to the value of P corresponding to the same control policy in Problem Π_0. This could also be expected from the fact that the state equations along the characteristics for Problem Π_e are identical to those for Problem Π_0 and by noticing that the $s_1 \times s_2$ domain converges smoothly to the $z \times t$ domain as $e \to 0$.

Table 4-2: Values of the objective functions P^* and P for the totally constrained policy k^* and the partly unconstrained policy $k^+(t)|_{\theta=0}$ as a function of θ.

θ	P^*	P
.150	.2813123	.2827461
.125	.2855542	.2872087
.100	.2900707	.2919824
.075	.2948736	.2970871
.050	.2999754	.3025444
.030	.3042804	.3071797
.020	.3065097	.3095913
.010	.3087915	.3120667
0.0	.3110862	.3146026

From these numerical results it follows that, for the case where the characteristics are not parallel to the lines along which the control would remain uniform, Problem Π_6 would constitute a counter-example for the strong maximum principle for boundary control if both of the following statements could be made:

1°: There exists an optimal piecewise continuous control $k^+(t) \in U$.

2°: $k(t) = k^*$ is the <u>best</u> totally constrained policy.

With regard to this second requirement, we can show rather easily that a totally constrained control where $k(t) = k_* = 0$ over a finite time interval $(t_1, t_2) \subset [0,1]$ with $t_2 - t_1 > e/(1+e)$ cannot be optimal. Indeed, from (4-54) and the geometry of the characteristic lines in Figure 4-11, this would imply that over the finite time interval $\Delta t = (t_1 + e/(e+1), t_2)$, the contribution to the objective function is zero. The value of the objective function then could be increased by letting $k(t) = k^*$ on Δt. However in case $t_2 - t_1 < e/(1+e)$, the characteristic lines s_1 which cross this time interval inside the $s_1 \times s_2$ domain become only partly inactive and the contribution to the objective function remains positive (Figure 4-11). Hence the case where a totally constrained control remains zero over a time interval $t_2 - t_1 \leq e/(1+e)$ needs further investigation.*

*Failure to realize this earlier resulted in an error in the discussion of the problem with nonorthogonal characteristics in our paper (Gruyaert and Crowe (1974)).

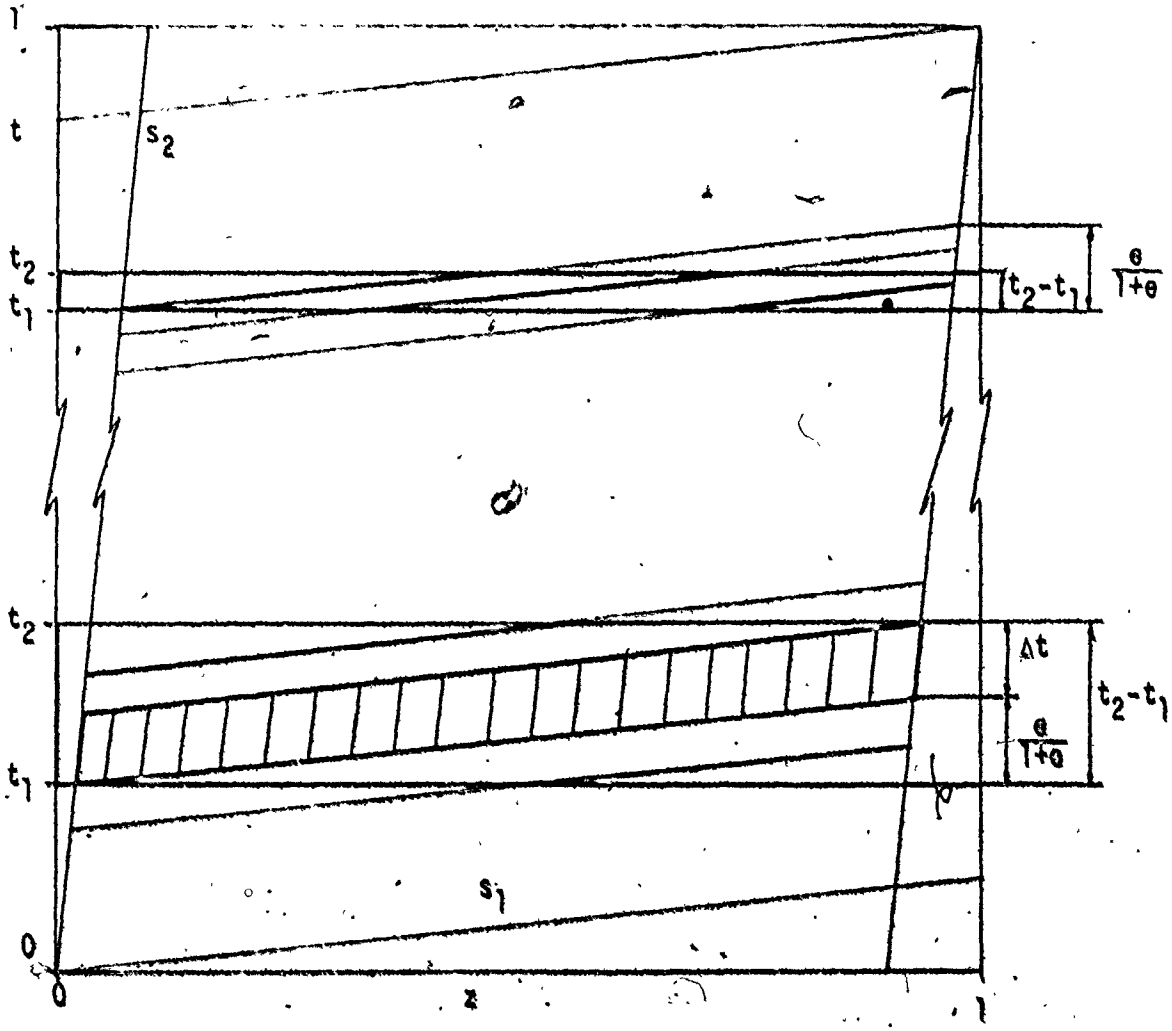

Figure 4-11: Partly inactive characteristics and region of total inactivity for $k(t) = 0$ over a finite time interval (t_1, t_2).

4.4.3 Relaxed Boundary Controls

Since for Problem Π_θ the characteristic lines s_1 are not parallel to the lines along which the control variable remains constant, it follows from the discussion under 4.3.7 that a relaxed boundary control $(\bar{K},\bar{k})$ as defined by (4-42) and (4-43) becomes a feasible controller. Since the boundary hamiltonian for Problem Π_θ was shown to be strictly convex with respect to k, we will consider a relaxed controller which chatters between the constraints k^* and k_*.

Consider now a particular type of bang-bang control policy which is constructed as follows:

1) Define

$$k(t) = \begin{cases} k^* \text{ for } t \in [t_1, t_2] \; ; \; t_2 > t_1 \\ \\ k_* \text{ for } t \in (t_2, t_3) \; ; \; t_3 > t_2 \end{cases}$$

2) Let

$$(t_3 - t_2) = (t_2 - t_1)$$

3) Starting at $t_1 = 0$, repeat 1) over N consecutive time intervals $[t_1, t_3)$, $(N < 1/(t_3 - t_1))$.

4) Define

$$k(t) = k^* \text{ for } t \in [N(t_3 - t_1), 1]$$

A sequence of such bang-bang control policies, defined on [0,1] for decreasing values of $(t_2 - t_1)$ and increasing values of N then converges

to a relaxed controller in the limit as $(t_2 - t_1) \to 0$ and $N \to \infty$.

For the given Problem $\prod_0$ with $t_f = 2.0$, calculations have been done for a sequence of bang-bang control policies of this type. In order to obtain the best accuracy in the numerical integration, a grid is constructed in the $s_1 \times s_2$ domain by dividing the s_1 characteristic into n equal parts and dividing the total time interval [0,1] into m equal time intervals Δt. It is most convenient to choose m as a multiple of n: $m = n \times q$ where q is an integer and to choose e such that $q(e/1+e) = 1$. This has the advantage that all points of intersection of s_1 and s_2 characteristics lie on lines parallel to the z-axis and that all sections of the $s_1 \times s_2$ domain enclosed by the s_2 characteristics and the horizontal lines through two consecutive grid points of the t-axis are identical. This grid structure for $n = 4$ and $q = 10$ $(e = 1/9)$ is illustrated in Figure 4-12. By choosing then the time interval $(t_2 - t_1)$, over which the bang-bang control policy remains at one of the constraints, equal to a multiple of Δt, the integration of the state equations can be carried out for consecutive horizontal sections. For each section Δt where $k(t) = k^*$, integration proceeds in the normal fashion along the characteristics s_1 and s_2. For the sections Δt where $k(t) = k_* = 0$, the values of the state variables x and ψ are carried along their appropriate characteristics without change.

Calculations have been done for the case with $e = 1/9$ and the grid structures $n = 8$ and $n = 20$. Since from 4.4.2, a controller where $(t_2 - t_1) > e/(1+e)$ cannot be optimal, only cases with $(t_2 - t_1) \leq 0.1$ will be considered. The numerical results are listed in Table 4-3. In order to make any

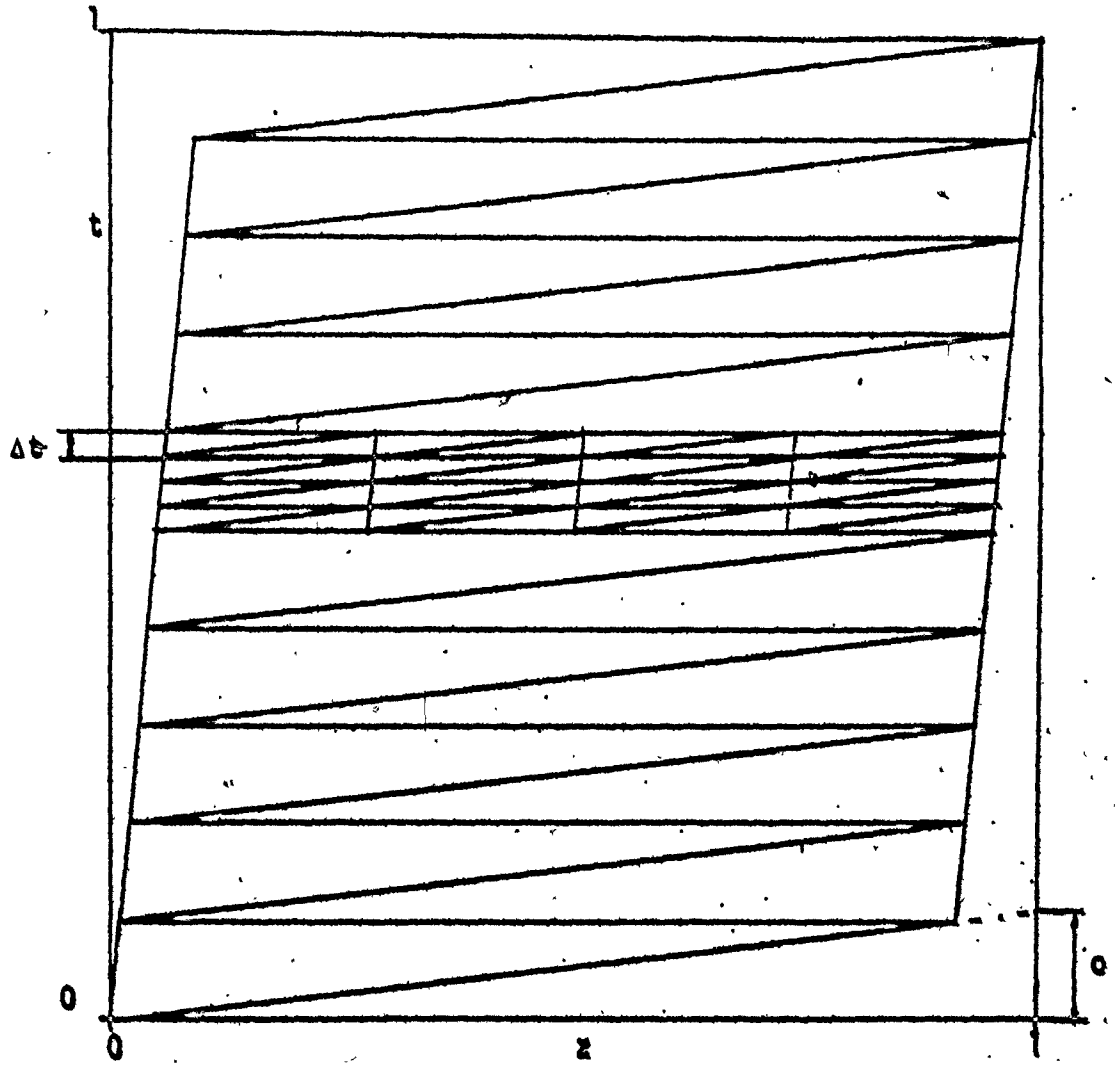

Figure 4-12: Grid structure used in the integration for Problem T_0 with $a = 1/9$ ($n = 4$, $q = 10$).

Table 4-3: Value of the objective function for a sequence of bang-bang control policies with $\epsilon = 1/9$.

Grid size n	$(t_2 - t_1)$	N	P
8	.1	4	.2886567
		3	.3005802
		2	.3050410
		1	.3015420
	.075	5	.3034842
		3	.3136044
		2	.3113714
		1	.3029543
	.05	6	.3170767
		4	.3102490
		2	.3007961
	.0375	10	.3069995
		7	.3160409
		4	.3130525
	.025	15	.3113172
		10	.3189178
		5	.3117605
		3	.3032999
	.0125	30	.3116633
		25	.3160260
		20	.3109512
		15	.3173630
		10	.3113005

continued

Table 4-3: Value of the objective function for a sequence of bang-bang control policies with $\epsilon = 1/9$ (continued).

Grid size n	$(t_2 - t_1)$	N	P
20	.01	30	.3176499
		25	.3189801
	.005	70	.3143378
		60	.3177102
		50	.3189874
		49	.3189929
		48	.3189761
		40	.3179496

conclusions based on the difference in the values obtained by using a smaller grid size (n = 20 compared with n = 8), the value of P^* where $k(t) = k^*$ for all $t \in [0,1]$ was calculated using both grid structures and showed a very high accuracy of the results: $P^*(n = 8) = .2880105$; $P^*(n = 20) = .2879893$. Linear interpolation between the values of P^* in Table 4-2 gives for $\theta = 1/9$: $P^* = .2880634$.

The value of P evaluated for the control $k^+(t)$, which was optimal for $\theta = 0$, was calculated for this case also with grid size n = 8 and gave: $P = .2898396$ (linear interpolation in Table 4-2 gives .2898607).

The following observations can now be made:

1°: For a given time interval $(t_2 - t_1)$ the value of the objective function shows a maximum with respect to N.

2°: As $(t_2 - t_1)$ decreases, the value of this maximum $P_{max}(t_2 - t_1)$ and $N_{max}(t_2 - t_1)$ are strictly monotonic increasing.

3°: The length of the time interval over which the control switches between k^* and $k_\#$ at P_{max} seems for any value of $(t_2 - t_1)$ to remain constant. This time interval is given by $2 \times N_{max} \times (t_2 - t_1)$ and lies in the neighbourhood of 0.5.

4°: The sequence of values of P_{max} as a function of $(t_2 - t_1)$ converges asymptotically towards a value P_R which would correspond to $t_2 - t_1 = 0$.

5°: The values of P_{max}, even for large time intervals $(t_2 - t_1)$, are considerably larger than P^* or $P(k(t) = k^+(t)$ for $e = 0)$.

From the numerical results in Tables 4-2 and 4-3, it seems unlikely that there would exist a piecewise continuous control, not totally constrained, which would give a value of the objective function larger than P_R. It is also interesting to mention that all attempts to find a stationary piecewise continuous policy for this problem have failed. By using a gradient method to 'hill-climb' on the boundary hamiltonian, and using different starting policies, the numerical search technique never converged to any solution.

One more point to consider is that the relaxed controller which is the limit of the sequence of bang-bang controllers used in our calculations, is not necessarily the best one for this problem. Indeed, by constructing a sequence of bang-bang controllers of a different type, it is quite likely that the corresponding values of P_{max} would converge to a different value of P_R in the limit since the sequence would converge to a different relaxed controller.

4.4.4 Conclusions

From the numerical results obtained for this particular Problem Π_2, we formulate the following hypotheses:

For the particular Problem Π_2 defined by (4-52) - (4-59) and with the set of parameters given by (4-22):

1) There exists an optimal relaxed controller, for any $e > 0$, which does not belong to the class of piecewise

continuous functions.

2) The sequence of optimal relaxed controllers for decreasing values of ϵ, converges smoothly to the infeasible optimal pseudo-relaxed controller for the corresponding Problem Π_0, as $\epsilon \to 0$.

3) The sequence of values of the objective function at the optimum for decreasing ϵ, converges smoothly to the value of P corresponding to the optimal pseudo-relaxed controller for Problem Π_0, as $\epsilon \to 0$.

This implies of course, that this particular Problem Π_0 does not constitute a counterexample for the strong maximum principle for boundary control since the problem does not allow an optimal admissible control to exist in the class of piecewise continuous functions.

Since in the proof of the strong maximum principle for boundary control, Chang required explicitly the presence of all partial derivatives of the state variables with respect to the independent variables in the state equations, and since the boundary control he used was a "uniform control" type, our Problem Π_0 would indeed not fit in this formulation. The maximum principle as formulated by Chang does imply that the lines along which the boundary control remains uniform are not parallel to any of the characteristic lines of the state equations. The maximum principle formulations given by Tarassov (1968), Butkovskii (1969) and Lovland (1972) are quite similar to the one used by Chang (1967), but none of these authors explicitly mention any requirements on the presence of all partial derivatives in the state equations. Butkovskii even

discusses an example in his book where the control remains uniform along one of the state characteristics (Butkovskii (1969, p60)).

In the work by Bykov et al. (1973, 1974a), however, the strong maximum principle for boundary control is formulated for problems where the state characteristics are also the lines along which the control remains uniform. They even went further and formulated also a strong maximum principle for the true boundary control problem where the control enters in the boundary conditions of the state equations.

Nishida et al. (1972) also state the strong form of the maximum principle, both for uniform and true boundary control, for distributed parameter problems where the characteristic lines coincide with the lines along which the control remains constant.

Because of the existence of a counter example in Problem Γ_0, these forms of the maximum principle, which apply to problems where the control remains uniform along one of the characteristics, are incorrect.

A counter example for the strong maximum principle for boundary control where the characteristics do not coincide with lines along which the control remains uniform has not been found up to date.

CHAPTER 5

CATALYTIC REACTOR SYSTEM

5.1 Tubular Fixed-Bed Catalytic Reactors

In the chemical and petrochemical industry, catalytic reactors are most commonly used because of the selective properties of a catalyst. Since in the chemical process industry, the reactants often consist of a mixture of many compounds which give rise to many side reactions, the selective property of a catalyst is used to change the rate of certain reactions, often a single reaction, leaving the rest unaffected. Catalytic reactors are then also widely used in many industrial processes. In this study, we will only consider solid catalyst and tubular fixed-bed reactors.

In order to describe a process, carried out in a tubular fixed-bed catalytic reactor, several mathematical models can be used. Froment (1970) has given an extensive review and classification of some of the most commonly used models. These models can be grouped into two classes, a first class of "pseudo-homogeneous models" which do not account explicitly for the presence of the catalyst as a separate phase, and a second class of "heterogeneous models" where separate equations are formulated for the fluid and solid phases. Both classes further contain one and two dimensional models, increasing in complexity and taking more effects into account.

Although the use of a "pseudo-homogeneous" model leads to a simpler set of equations, the correspondence of the real system and the

model depends upon how completely the effects of the solid phase can be included in the homogeneous equations (Petersen (1965)). For fixed-bed reactors where the heat and mass transfer between the fluid phase and the catalyst particles is very rapid and when the size of the catalyst particles is small in comparison to the dimensions of the reactor, a "pseudo-homogeneous" model is reasonably justifiable.

The basic assumptions which we will use are:

- At any point inside the reactor, both the solid and fluid phase are considered to be at equivalent equilibrium stages. This means that there are no effective temperature and concentration gradients between the fluid and the catalyst particles at any point in the reactor.
- Bulk flow is along the axis of the reactor only (z-direction).
- Axial diffusion and radial concentration gradients are negligible.

If we further assume that the density of the fluid phase can be taken as constant for the range of operating conditions, the continuity equation in terms of molar units for a component i in some reactor element may be written as:

$$\frac{\partial c_i}{\partial t} + v \frac{\partial c_i}{\partial z} = R_i \qquad (5\text{-}1)$$

where c_i is the molar concentration of species i, v is the molar average velocity along the axis of the reactor, and R_i is the molar rate of formation of species i. The independent variables are t, the chronological

time since start-up of the reactor: $t' \in [0, t_f]$ where t_f is total operating time, and z', the distance along the axis of the tubular reactor: $z' \in [0, L]$ where L is the total length of the catalyst bed.

For a single chemical reaction, the rate of reaction R_i can be expressed as a function of temperature T, chemical conversion x and relative catalyst activity ψ:

$$R_i = \Omega[T, x, \psi] \tag{5-2}$$

Since the mechanisms of catalytic reactions are complex phenomena, the rate expressions which can be derived from theoretical considerations are usually very complicated. Moreover, this type of approach often leads to a large number of possibilities and it is not always easy to choose a particular rate expression. An example with 23 possible rate expressions for the ammonia synthesis reaction is given in a paper by Ferraris et al. (1974).

Rather than trying to describe exactly the mechanism of the reaction we can make use of a pseudo-homogeneous rate of reaction which is of a much simpler form. It has been shown in the literature (see Prater and Lago (1956)) that in terms of the contact time or space time, most catalytic conversion data can be fitted adequately by simple first- or nth-order rate expressions. Weller (1956, 1974) has also shown that reaction rate expressions derived in this manner are compatible with much more complex forms and that in some cases, they are even better representations.

In the course of this study, the pseudo-homogeneous rate of

reaction of an irreversible reaction A → B will be expressed as a product of separate functions each depending on only one of the state or decision variables:

$$\Omega[T,x,\psi] = K'[T] \cdot F[x] \cdot \psi \qquad (5\text{-}3)$$

In terms of the conversion x, (5-1) can then be rewritten as

$$\frac{\partial x_T}{\partial t} + v \frac{\partial x_T}{\partial z} = K'[T] \cdot F[x] \cdot \psi \qquad (5\text{-}4)$$

The function $K'[T]$ is assumed to be of the Arrhenius form and then is a positive continuous strictly monotonic increasing and differentiable function of the temperature $T(z',t')$:

$$K'[T] = K_0 \exp(-E_R/R/T) \qquad (5\text{-}5)$$

where K_0 and R are constants and E_R is the reaction activation energy.

The function F[x] is considered a continuous monotonic decreasing function of the conversion $x(z',t')$, or a constant, such that

$$0 \leq x(z',t') \leq 1 \qquad (5\text{-}6)$$

implies

$$0 \leq F[x] \leq 1 \qquad (5\text{-}7)$$

Furthermore F[x] is assumed to be twice continuously differentiable with respect to its argument.

The effectiveness of the catalyst is expressed in terms of the relative catalyst activity $\psi(z',t')$ and is defined as

$$\psi(z',t') = \frac{\text{rate of reaction using catalyst in a given condition}}{\text{rate using fresh catalyst or catalyst in a reference state}} \tag{5-8}$$

Defining the relative effectiveness of the catalyst in this manner eliminates the necessity of considering the combined effects of operating conditions, structure of the catalyst, contacting mechanisms and the kinetics (Anderson (1968)).

The initial and boundary conditions for Equation (5-4) are

$$x(o,t') = x_o(t') \tag{5-9}$$

and

$$x(z',o) = x_o(z') \tag{5-10}$$

where $x_o(t')$ and $x_o(z')$ are given and may in general be piecewise continuous functions of t' and z' and have piecewise continuous first derivatives with respect to t' and z' along their respective boundaries of the domain $[o,t_f]x[o,L]$.

In most of the tubular fixed-bed reactors, the space time (time required for a fluid element to pass through the reactor) is small (seconds or minutes) in comparison with the total operating time of the reactor (hours or days). Under most circumstances, the change in relative catalyst activity over a time interval equal to the space time is nearly negligible. If this is the case and if

$$\frac{\partial X}{\partial t}_{T} << v \frac{\partial X}{\partial z}_{t} \qquad (5\text{-}11)$$

at any point in the domain of definition (Therien (1971, Appendix F)), the quasi-steady state approximation can be used and Equation (5-4) can be written as

$$v \frac{\partial X}{\partial z}_{T} = K^{\dagger}[T].\ F[x]\ .\ \psi \qquad (5\text{-}12)$$

with the natural boundary condition (5-9).

5.2 Catalyst Deactivation

The loss of catalyst activity during a reaction is a very complicated phenomenon, mainly due to the fact that there can be many causes for the deactivation. Some of the many forms of decay which are commonly encountered are sintering of the catalyst, deposition of poisons or reaction-residues on active-sites and pore plugging by poisons or reaction-residues in the feed- or product stream.

In order to model the deactivation process, two main directions can be followed, A first approach is to characterize the state of the catalyst at each point inside the reactor. An example of this has been given by Froment and Bischoff (1961,1962) who tried to formulate a model relating the activity to the coke-on-catalyst. The major disadvantage of such an approach is of course, the difficulty of taking quantative measurements during the course of an experimental run. A second type of decay model has been derived from the Time On Stream Theory as developed by Wojciechowski (1968). This approach is based on integral measures of the

state of the catalyst in the reactor only and leads to a model for deactivation of the catalyst as a function of time, but averaged over the whole reactor. The time on stream theory has recently been shown to be efficient in modelling the catalyst decay for cracking reactions (John, Pachovsky and Wojciechowski (1974)). In this paper, the author also points out the discrepancy between his approach and the models derived by relating the activity to coke-on-catalyst. A comprehensive review of the Time On Stream Theory was recently published by Wojciechowski (1974).

The catalyst deactivation model which will be used in this study is the one proposed by Szepe (1966). The simple but theoretically acceptable form for the rate of deactivation is similar to the rate expression for a chemical reaction and is defined as the product of separate functions of the operating and catalyst condition,

$$\text{rate of deactivation} = -k^{\dagger}[T] \cdot f[x] \cdot g[\psi] \tag{5-13}$$

with $g[\psi]$ of the power form:

$$g[\psi] = \psi^{m} \tag{5-14}$$

and $k^{\dagger}[T]$ is of the Arrhenius form:

$$k^{\dagger}[T] = k_{o} \exp(-E_{c}/R/T) \tag{5-15}$$

where k_o and R are constants and E_c is the activation energy for decay. The parameter m in (5-14) is called the order of deactivation. The function f[x] expresses the conversion dependence of the catalyst decay rate.

Szepe (1966) also showed the linear, exponential and hyperbolic forms of decay models, obtained on the basis of experiments, all to be special cases of (5-13) with $g[\psi]$ given by (5-14). Further support for this model form can be found in the work by Szepe and Levenspiel (1968a,b), Khang (1971), Levenspiel (1972), Dougharty (1970), Blaum (1974). A review of this type of catalyst decay models has been given by Butt (1972).

This however does not exclude the occurrence of more complex deactivation processes for which (5-13) is no longer an adequate representation (Wheeler and Robell (1969), Bakshi and Gavalas (1973)). Nevertheless, the rate expression (5-13) can often be used as a first approximation to many such complex deactivation processes.

For the purpose of this study, we will use the following rate expression for the catalyst decay

$$\frac{\partial \psi}{\partial t} = - k^{\dagger}[T]\, f[x]\, \psi^{m} \qquad (5\text{-}16)$$

which expresses the rate of change of the relative catalyst activity $\psi(z',t')$ as a function of temperature, conversion and relative catalyst activity at each point (z',t') of the domain of definition $[o,t_f]x[o,L]$. The function $f[x]$ is assumed to be a non-negative continuous function of its argument, or a constant, and is considered to be twice continuously differentiable with respect to x.

In addition to (5-16) we define the natural boundary condition as

$$\psi(z',o) = \psi_o(z') \qquad (5\text{-}17)$$

where $\psi_o(z')$ is a piecewise continuous function with piecewise continuous first derivatives with respect to z' along this boundary of the domain.

5.3 Formulation of the Optimization Problem

By defining the following transformations

$$z = z'/L \tag{5-18}$$

$$t = t'/t_f \tag{5-19}$$

$$K[T] = t_f\, K'[T] \tag{5-20}$$

and

$$k[T] = t_f\, k'[T] \tag{5-21}$$

the variables z e[o,1], t e[o,1], K[T] and k[T] are all made dimensionless.

With $t_\theta = L/v$, the unsteady state catalytic reactor system may then by written as

$$x_t + \left(\frac{t_f}{t_\theta}\right) x_z = K[T]\, F[x]\, \psi \tag{5-22}$$

and the quasi-steady state system,

$$\left(\frac{t_f}{t_\theta}\right) x_z = K[T]\, F[x]\, \psi \tag{5-23}$$

with the equation for the deactivation:

$$\psi_t = -\, k[T]\, f[x]\, \psi^m \tag{5-24}$$

The corresponding initial and boundary conditions to these partial differential equations are:

$$x(o,t) = x_o(t) \tag{5-25}$$

$$x(z,o) = x_o(z) \tag{5-26}$$

$$\psi(z,o) = \psi_o(z) \tag{5-27}$$

Because of the equivalence in the state equations between most adiabatic reactors and a reactor where the temperature is uniform (Appendix A), we will only consider problems where the temperature T is a function of t only. This means that the temperature T(t) remains constant along the axis of the reactor for a uniform temperature reactor where T(z,t) = T(t) and refers to the inlet temperature into the reactor at z = 0, $T_o(t)$, for an adiabatic reactor.

Since by assumption K[T] and k[T] are both of Arrhenius form, it follows form (5-5),(5-15), (5-20) and (5-21) that

$$K[T] = A.(k[T])^p \tag{5-28}$$

with

$$A = t_f \cdot K_o/(t_f \cdot k_o)^p \tag{5-29}$$

where p is the ratio of the activation energy for reaction E_R to the deactivation energy E_c:

$$p = E_R/E_c \tag{5-30}$$

The performance of the catalytic reactor system will be measured as the amount of reaction which was obtained over the total operating period and is given by:

$$P = \int_0^1 [x(1,t) - x_0(t)]dt \qquad (5\text{-}31)$$

5.3.1 Boundary Control Alternatives

For the quasi-steady state problem (5-23), (5-24) with initial and boundary conditions (5-25), (5-27), an optimization problem can then be defined as: "Maximize the objective function P over all admissible control policies".

Since we deal with boundary controls only, possible control variables for this reactor system are:

- Inlet temperature of the fluid into the reactor as a function of time.
- Composition of the feed stream into the reactor as a function of time.
- Distribution of the relative catalyst activity along the reactor axis at initial time.
- Velocity of the fluid stream through the reactor as a function of time.

Although they are not real boundary controls as defined in this study, the length of the catalyst bed and the total operating time can also be defined as control variables.

From physical considerations, the control variables will usually be required to lie in an admissible control region.

For the given optimization problem, the following boundary controls and combinations of these will now be further investigated:

- Inlet temperature $T(t)$.
- Initial relative catalyst activity distribution $\psi_0(z)$.
- Fluid flow rate $v(t)$.

CHAPTER 6

INLET TEMPERATURE CONTROL

6.1 Problem Formulation

By dividing both sides of the partial differential equation (5-23) by the factor (t_f/t_θ) and absorbing this factor into the proportionality constant A (Equation 5-28), the quasi-steady state expressions for an irreversible catalytic reaction can more conveniently be written as

$$x_z = K[T]F[x]\psi \tag{6-1}$$

The equation expressing the rate of the catalyst decay is

$$\psi_t = - k[T]f[x]g[\psi] \tag{6-2}$$

Where the function $g[\psi]$ will usually take on the form $g[\psi] = \psi^m$. Initial and boundary conditions to (6-1) and (6-2) are

$$x(o,t) = x_o(t) \qquad t \in [o,1] \tag{6-3}$$

$$\psi(z,o) = \psi_o(z) \qquad z \in [o,1] \tag{6-4}$$

The boundary control variable T(t), which is the inlet temperature into the tubular reactor, will be required to lie between an upper and lower constraint :

$$T_* \leq T(t) \leq T^* \quad \text{all } t \in [0,1] \tag{6-5}$$

where T_* and T^* will be considered constant.*

Since $K[T]$ is proportional to $(k[T])^P$ and since $k[T]$ is a strictly monotonic increasing function of T, the function $k[T]$ can be treated as the control variable $k(t)$. The constraints k_* and k^* for $k(t)$ can be calculated from (6-5) as

$$k[T_*] = k_* \leq k(t) \leq k^* = k[T^*] \tag{6-6}$$

The optimal boundary control problem for the system (6-1)-(6-4) then becomes: Choose a piecewise continuous function $k^+(t)$ which satisfies (6-6) such that the objective function P,

$$P = \int_0^1 [x_1(t) - x_0(t)]dt \tag{6-7}$$

reaches an absolute maximum with respect to all admissible piecewise continuous controls $k(t)$.

6.2 Application of the Maximum Principle for Boundary Control

For the given optimal control problem, the hamiltonian function

*In adiabatic reactors, where upper and lower constraints are placed on the temperature inside the reactor: $T_{min} \leq T(z,t) \leq T_{max}$, the constraints T_* and T^* on the inlet temperature $T_0(t)$ will become functions of t through the state variables and can be calculated from T_{min} and T_{max}.

can be defined as

$$H = \lambda K F \psi - \mu k f g \tag{6-8}$$

where the adjoint variables λ and μ are the solutions of

$$\lambda_z = - \lambda K F' \psi + \mu k f' g \tag{6-9}$$

$$\mu_t = - \lambda K F + \mu k f g' \tag{6-10}$$

with terminal and boundary conditions:

$$\lambda(1,t) = 1 \quad \text{all } t \in [0,1] \tag{6-11}$$

$$\mu(z,1) = 0 \quad \text{all } z \in [0,1] \tag{6-12}$$

The functions F', f' and g' in (6-9) and (6-10) denote the first derivatives of F, f and g with respect to their respective dependent variables x or ψ.

The boundary hamiltonian $\bar{H}$ is given by

$$\bar{H} = \int_0^1 H dz \tag{6-13}$$

Application of the weak maximum principle for boundary control then leads to the following necessary conditions for optimality.

In order for an admissible control $k^+(t)$ to be optimal it is necessary that:

$$\left.\frac{\partial \bar{H}}{\partial k}\right|_{k^+(t)} = 0 \text{ whenever } k_* < k^+(t) < k^* \tag{6-14}$$

$$\left.\frac{\partial \bar{H}}{\partial k}\right|_{k^+(t)} \geq 0 \text{ when } k^+(t) = k^* \tag{6-15}$$

$$\left.\frac{\partial \bar{H}}{\partial k}\right|_{k^+(t)} \leq 0 \text{ when } k^+(t) = k_* \tag{6-16}$$

The necessary conditions (6-14)-(6-16) can also be derived from a first order perturbation analysis of the objective function P (Appendix B). The optimal control policies corresponding to (6-14), (6-15) and (6-16) will be denoted as S, C^* and C_* policies respectively.

6.3 Properties of the Optimal Control ($f(x) \neq$ constant)

Although any piecewise continuous control function can be constructed from a combination of S, C^* and C_* policies, it has been shown that for the conversion independent decay problem, the optimal inlet temperature policy can only consist of certain combinations of the three types of policies (Crowe (1970)). Similar results were also obtained by Therien (1971) for the conversion independent decay problem with distributed temperature control. In both these studies, it was shown that the value of the parameter p, defined in (5-30), plays a decisive role in determining the admissibility of certain control policies to be the optimal control policy. In the conversion independent decay problems studied by Crowe and Therien, it also could be shown that, under certain conditions, any optimal control policy which contained a sub-policy

S needed also to be continuous. In the present study where we consider the catalyst decay to be conversion dependent, two major complications arise.

A first difficulty arises from the influence of the conversion dependent factor $f(x)$ in the decay rate expression (6-2) on the nature of the optimal control policy. Indeed, since for values of $p < 1$, the rate constant for decay $k[T]$ increases faster than the reaction rate constant $K[T]$, it would not always seem desirable to work at the highest possible temperature T^*. Because of this, it was possible to prove that, for the case where $f(x) =$ constant, an admissible control policy which contains a stationary sub-policy S is a feasible policy for optimality. If now however, $f(x) \neq$ constant and if $f(x)$ is a decreasing function of x, the greater rate at which the catalyst decays at higher temperatures can possibly be offset by a decrease in $f(x)$ which in turn is due to the higher attained conversion at higher temperatures. Therefore, we can see intuitively that there can exist problems where a sub-policy S can never be part of the optimal policy for $p < 1$ provided $f' < 0$. Similarly, it could be proven that for problems with $p > 1$ and $f(x) =$ constant, except under certain special circumstances, (Crowe (1970)), the sub-policy S never could be part of the optimal control policy. Although for $p > 1$, the reaction rate constant increases faster with temperature than the rate constant for decay, the catalyst still could be made to decay faster under the influence of increased conversion through $f(x)$. Hence, even for $p > 1$, an optimal policy which contained a sub-policy S could indeed become feasible.

A second complication, and a much more drastic one, is the fact that for the given quasi-steady state problem under consideration, a strong maximum principle has been proven not to exist (see Chapter 4). Since in the derivations of the optimal control properties for problems with conversion independent decay, extensive use could be made of a strong maximum principle formulation, these proofs cannot in general be extended to prove similar properties of the optimal control for our problem.

Some of the properties which still can be proven for the problem with $f(x) \neq$ constant will now be summarized. Trivial situations where the initial catalyst activity distribution $\psi_0(z)$, $z \in [0,1]$ is identically zero or where the inlet conversion $x_0(t)$, $t \in [0,1]$ is the maximum attainable conversion in the reactor will be ignored. We also will consider only problems where the relative catalyst activity at the end of the operation $\psi_1(z)$, $z \in [0,1]$, still has a positive value. The case where $p = 1$ and which leads to the study of singular controls has not been treated in this work. We also recall that in 5.1, we assumed $F(x)$ to be a monotonic decreasing function of x, which means that autocatalytic reactions($F' > 0$) are excluded.

We wish to reiterate that all properties discussed below which apply to the optimal policy apply to a given control problem only, when an optimal control policy does exist for that problem.

Property 1:

$$k^+(t) = k^* \quad \text{for } t \in (1 - \delta t, 1]$$

Proof:

From (6-9), (6-11) and (6-12) follows

$$\lambda(z,1) > 0 \qquad \text{all } z \in [o,1] \tag{6-17}$$

Since

$$\frac{\partial \bar{H}}{\partial k} = \int_0^1 (P \frac{\lambda K}{k} F \psi - \mu f g) dz \tag{6-18}$$

it follows from (6-12) and (6-17) that with $\psi(z,1) > 0$,

$$\frac{\partial \bar{H}}{\partial k}\Big|_{t=1} > 0 \qquad \text{for all } k \in [k_*, k^*] \tag{6-19}$$

Hence the only value of the control which can satisfy the necessary conditions (6-14)-(6-16) at $t = 1$ is k^*. From (6-2) and (6-10) follows that ψ and μ are continuous functions of t. Since $\partial \bar{H}/\partial k$ is a continuous function of its arguments and since $x_0(t)$ and $k(t)$ are piecewise continuous, (6-19) implies that there exists a finite time interval $\delta t > 0$ such that $\partial \bar{H}/\partial k$ remains positive for all values of $k \in [k_*, k^*]$ over the time interval $(1 - \delta t, 1]$. Hence the only control which can satisfy (6-14)-(6-16) is $k^+(t) = k^*$ for $t \in (1 - \delta t, 1]$. Q.E.D.

Property 2:

$f' < 0$ implies $\lambda(z,t) > 0$ for all $z \in [0,1]$ all $t \in [o,1]$

Proof:

For the proof of this property, the same arguments can be used as in Appendix E. The only difference for this problem is that the characteristic lines are orthogonal and coincide with the coordinate axes.

Remark:

Although in all our numerical work we never encountered a problem where λ became nonpositive, the same procedure cannot be used to prove that λ remains positive over the whole domain when $f' > 0$.

Property 3:

$\bar{H}$ is strictly concave for $f' < 0$ and $0 < p < 1$ and is strictly convex for $f' < 0$ and $p > 1$.

Proof:

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

$$\frac{\partial^2 \bar{H}}{\partial k^2} = \int_0^1 p(p-1) \frac{\lambda K F \psi}{k^2} dz \qquad (6\text{-}20)$$

this property follows directly from Property 2. Q.E.D.

Property 4:

> For $f' < 0$, a stationary control policy S is an admissible control sub-policy to the optimal control policy.

Proof:

Since $\partial^2\bar{H}/\partial k^2$ is strictly negative for $0 < p < 1$ and strictly positive for $p > 1$, it is clear that $\bar{H}$ can exhibit a stationary point for some $k \in (k_*, k^*)$. This is a sufficient condition for a control which is unconstrained over a finite time interval to be an admissible control for optimality. Because of Property 1, a totally unconstrained policy S however, cannot be optimal. Q.E.D.

Property 5:

> For $f' < 0$ and $0 < p < 1$, any control policy which satisfies the necessary conditions of the maximum principle for boundary control is uniquely determined at each $t \in [o,1]$.

Proof:

From Property 3, we have that for $f' < 0$ and $0 < p < 1$, $\bar{H}$ is strictly concave with respect to $k \in [k_*, k^*]$. As illustrated in Figure 6-1, only three types of functions $\bar{H}$ vs. k are possible at each $t \in [o,1]$. The property follows then from the fact that for each of the three possibilities,

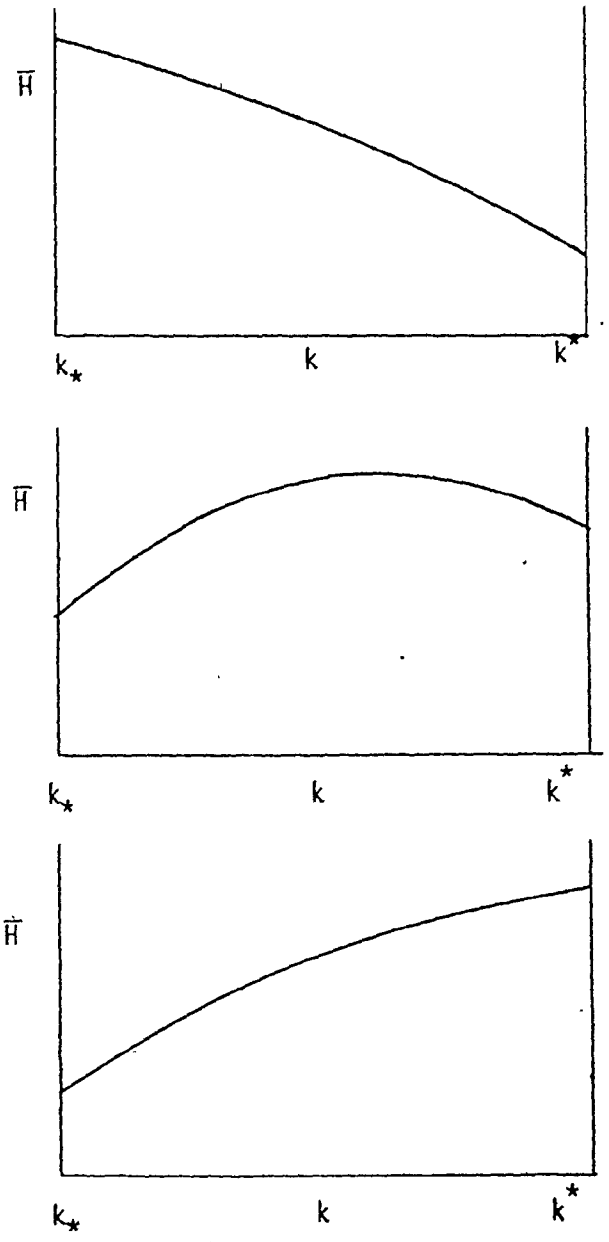

Figure 6-1: Typical curves of the function $\bar{H}$ vs. k, $k \in [k_*, k^*]$, for $f' < 0$ and $0 < p < 1$.

there is only one value of k for which one of the necessary conditions (6-14) - (6-16) can be satisfied. Q.E.D.

Remark 1:

Note that although $\bar{H}$ is strictly convex with respect to k for $f' < 0$ and $p > 1$, no specific properties of the optimal control can be derived in this case.

Indeed since we cannot use any strong form of the maximum principle, there are three values of k for which the necessary conditions (6-14) - (6-16) can be satisfied whenever $\bar{H}$ has a minimum inside the admissible control region.

Remark 2:

Although most properties could be derived for the case where $f' < 0$ and $0 < p < 1$, we have not been able to prove that an optimal control policy which contains an unconstrained sub-policy S also needs to be continuous. Indeed, the fact that $f(x) \neq$ constant does not seem to make it possible to contradict the conditions which must be satisfied whenever a finite jump in the control values occurs.

6.3.1 The Constant Exit Conversion Property

The constant exit conversion property which states that: "The exit conversion $x_1(t)$ remains constant over any finite time interval where the optimal control policy $k^+(t)$ is unconstrained, provided $x_0(t)$ remains constant over that time interval", has first been proven by Szepe (1966)

for conversion independent decay problems ($f' = 0$).

A similar property has also been proven for the problem with conversion dependent decay ($f' \neq 0$), but with distributed temperature control $k(z,t)$, by Crowe (1975). Although up to this date we have not been able to prove this property for the given boundary control problem with general kinetics and $f' \neq 0$, the constant exit conversion property was proven to be valid for the class of problems where $F = 1 - x$, $f = (1 - x)^r$ and $g = \psi$. This class of problems was encountered in the discussion of Problem Π_0 in Chapter 4. The constant exit conversion was discussed there as Property 2 and the proof for all values of r ($r \neq 0$), $p \neq 1$) is given in Appendix D. Since in the study of the counter example in Chapter 4, a more general notation form was used, the variable f which appears in the lumped version of Problem Π_0 and also in Appendix D corresponds with the exit convefsion $x_1(t)$ in the present formulation of the problem.

The constant exit conversion property has also been proven for the class of problems: $F = (1 - x)^2$, $f = (1 - x)^r$, $g = \psi$ for all values of r ($r \neq 0$, $p \neq 1$), and for the class of problems where $F = 1 - x$, $f = x$, $g = \psi$. The proofs for this latter two classes of problems will not be given here, but they follow essentially the same pattern as the proof in Appendix D. The boundary control problems are first transformed into a lumped parameter problem. The maximum principle of Pontryagin is then applied to this lumped problem and an expression similar to (D-9) is obtained. Although the terms in this expression vary for the different classes of problems, the common characteristics remain the same. Either

dx_1/dt is zero or a function which multiplies this time derivative has to vanish over that time interval where the optimal control is unconstrained. This then is used to establish that $dx_1/dt = 0$ on S is the only possibility at the optimum provided of course that $dx_o/dt = 0$ on S and that the control is continuous over that time interval.

The common factor in these three classes of conversion dependent decay problems is of course that all of them are first-order decay rate problems ($g = \psi$). Another observation which was made in these proofs was that the expression (D-8), which was extremely useful in the proof in Appendix D, reappeared in exactly the same form in the proofs for the other classes of problems, notwithstanding the fact that the lumped system equations were totally different in each class of problems. It is primarily this last observation which led us to the following proof of the constant exit conversion property for first-order decay rate problems with otherwise quite general kinetics.

Property 6:

Given the following conditions:

(i) $g = \psi$

(ii) $0 < p < 1$ or $p > 1$

(iii) F is a continuous function of x and nonzero for all $x \in [x_o, x_1]$

(iv) f is a continuous function of x

(v) $k^+(t)$ is unconstrained and continuous over a finite time interval $(t_1, t_2) \subset [o, 1]$

(vi) $x_o(t)$ is <u>constant</u> for $t \in (t_1, t_2)$

then

$$\frac{dx_1(t)}{dt} = 0 \quad \text{for all } t \in (t_1, t_2)$$

<u>Comment:</u>

The condition that $F \neq 0$ is not a very severe one. It mainly excludes autocatalytic reactors where $x_o(t) = 0$ and reactors where complete conversion is reached. Since we have been unable to prove that no finite switches in the unconstrained optimal control policy can occur, we have to assume continuity of $k^+(t)$ on S.

<u>Proof:</u>

Since $F \neq 0$, we can write (6-1) as

$$\frac{dx}{F} = K \psi dz \tag{6-21}$$

and since 1/F is integrable

$$\int_{x_o}^{x'} \frac{dx'}{F} = K \int_o^{z'} \psi dz \qquad z' \in [o,1] \tag{6-22}$$

Defining

$$\phi' = \int_o^{z'} \psi dz \tag{6-23}$$

we can write (6-22) as

$$F_1(x_0,x) = K\phi' \tag{6-24}$$

where F_1 is a continuously differentiable function of x_0 and x. Defining $\phi = \phi'$ at $z' = 1$ we get

$$F_1(x_0,x_1) = K\phi \tag{6-25}$$

Since

$$\frac{\partial F_1}{\partial x} = \frac{1}{F} \neq 0 \tag{6-26}$$

we can apply the implicit function theorem and (6-24) can be written as

$$x = F(x_0,K\phi') \tag{6-27}$$

where F is continuously differentiable with respect to x_0 and $K\phi'$. Since $x_0(t)$ is assumed constant on S, we will not consider x_0 as a dependent variable, hence

$$x = F(K\phi') \tag{6-28}$$

and

$$x_1 = F(K\phi) \tag{6-29}$$

Substituting (6-28) into (6-2) and integrating over z gives:

$$\int_0^1 \psi_t dz = - k \int_0^1 g_1(K\phi')\psi dz \tag{6-30}$$

where

$$g_1(K\phi') = f[F(K\phi')] \tag{6-31}$$

is a continuous function of $K\phi'$.

From the definition of ϕ' (6-23), Equation (6-30) can be written as

$$\frac{d\phi}{dt} = - \frac{k}{K} \int_0^{K\phi} g_1(K\phi')dK\phi' \tag{6-32}$$

Since g_1 is continuous, the integral in (6-32) exists and we get

$$\frac{d\phi}{dt} = - \frac{k}{K}\ g(K\phi) \tag{6-33}$$

where

$$g(K\phi) = \int_0^{K\phi} g_1(K\phi')dK\phi' \tag{6-34}$$

is a continuously differentiable function of $K\phi$. The initial condition to (6-33) is given by

$$\phi_o = \phi(o) = \int_0^1 \psi_o(z)dz \tag{6-35}$$

The optimization problem is then

$$\max_{k_* \leq k(t) \leq k^*} P = \max_{k_* \leq k(t) \leq k^*} \int_0^1 F(K_\phi)dt \tag{6-36}$$

with the state equation given by (6-33) and initial condition (6-35). We now can apply the maximum principle of Pontryagin to this lumped problem.

The lumped hamiltonian function H_ℓ is defined as:

$$H_\ell = F(K\phi) - \frac{\gamma k}{K} g(K\phi) \tag{6-37}$$

with

$$\frac{d\gamma}{dt} = - \frac{\partial H_\ell}{\partial \phi} \tag{6-38}$$

and

$$\gamma(1) = 0 \tag{6-39}$$

The necessary conditions for optimality can then be written as

$$\frac{dH_\ell}{dt} = 0 \quad \text{for all } t \in [o,1] \tag{6-40}$$

$$k \frac{\partial H_\ell}{\partial k} = 0 \quad \text{on } S \tag{6-41}$$

With H_ℓ given by (6-37) these conditions can be expressed as:

$$\frac{dH_\ell}{dt} = (F' - \frac{\gamma k}{K} g') \frac{dK\phi}{dt} - g \frac{d(\gamma k/K)}{dt} = 0 \quad \text{for } t \in [o,1] \tag{6-42}$$

and

$$k \frac{\partial H_\ell}{\partial k} = F' pK\phi - \frac{\gamma k}{K} ((1 - p)g + g' pK\phi) = 0 \text{ on } S \tag{6-43}$$

where F' and g' denote the partial derivatives of F and g with respect to

K_ϕ respectively.

Since $g \neq 0$ ($g = 0$ would imply $k = 0$ or $\phi = 0$ and these can be excluded), Equation (6-42) can be written as

$$\frac{d(\gamma k/K)}{dt} = \frac{F' - (\gamma k/K)g'}{g} \frac{dK_\phi}{dt} \qquad \text{all } t \in [o,1] \tag{6-44}$$

Since γ is a solution of (6-38) with terminal condition (6-39), γ is a continuous function of t for all $t \in [o,1]$. The factor which multiplies $(\gamma k/K)$ in (6-43) then cannot become zero on S since from (6-43) this would imply that $F' = 0$. (the possibilities of $k = 0$ or $\phi = 0$ are excluded). However, from (6-29) and (6-21), $F' = 0$ would imply that $F(x_1)$ is zero and this has been excluded.

Hence from (6-43) we obtain

$$\frac{\gamma k}{K} = \frac{F' pK_\phi}{(1 - p)g + g' pK_\phi} \qquad \text{on S} \tag{6-45}$$

Substituting (6-45) into (6-44) gives:

$$\frac{d(\gamma k/K)}{dt} = \frac{F'(1 - p)}{(1 - p)g + g' pK_\phi} \cdot \frac{dK_\phi}{dt} \quad \text{on S} \tag{6-46}$$

or with (6-45)

$$\frac{d(\gamma k/K)}{dt} = \frac{\gamma k}{K} \left(\frac{1 - p}{p}\right) \frac{1}{K_\phi} \frac{dK_\phi}{dt} \quad \text{on S} \tag{6-47}$$

and this gives after integrating

$$\frac{\gamma k}{K} = \alpha (K_\phi)^{(1-p)/p} \quad \text{on S} \tag{6-48}$$

where α is a constant.

Substituting (6-48) into (6-37) gives from (6-40) the following necessary condition on S:

$$H(K\phi) = F - \alpha(K\phi)^{(1-p)/p} g - C = 0 \quad \text{on } S \tag{6-49}$$

where C is a positive constant.

We now have the following possibilities for $K\phi$ on S:

$$1) \quad \frac{dK\phi}{dt} = 0 \quad \text{for all } t \in (t_1, t_2) \tag{6-50}$$

$$2) \quad \frac{dK\phi}{dt} \neq 0 \quad \text{for } t \in (t_a, t_b) \subseteq (t_1, t_2) \tag{6-51}$$

From (6-29) we have

$$\frac{dx_1}{dt} = F'(K\phi) \frac{dK\phi}{dt} \tag{6-52}$$

and hence since $F' = 0$ can be excluded, (6-50) implies

$$\frac{dx_1}{dt} = 0 \quad \text{on } S \tag{6-53}$$

in which case the constant exit conversion property holds. Since from (6-33) and (6-35) it follows that ϕ is a continuous function of t, and since we assumed the optimal control to be continuous on S, $K\phi$ is also a continuous function of t on S. Equation (6-51) then implies that $K\phi$ attains all values

$$K\phi \in (\underline{K\phi}, \overline{K\phi}) \tag{6-54}$$

on the open time interval (t_a, t_b), where

$$\underline{K\phi} = \min[K\phi(t) | t_a \leq t \leq t_b] \tag{6-55}$$

and

$$\overline{K\phi} = \max[K\phi(t) | t_a \leq t \leq t_b] \tag{6-56}$$

with $\overline{K\phi} > \underline{K\phi}$. This further implies that for all $K\phi \in (\underline{K\phi}, \overline{K\phi})$ on (t_a, t_b), the necessary condition (6-49) needs to be satisfied. However, since F and g are differentiable with respect to $K\phi$, the function $H(K\phi)$ is analytic and hence has only isolated roots. Therefore, since $\overline{K\phi} > \underline{K\phi}$, it is impossible to satisfy (6-49) for all values of $K\phi \in (\underline{K\phi}, \overline{K\phi})$. This means that condition (6-51) can never occur. Q.E.D.

Since for $g = \psi^m$ with $m \neq 1$, the system equations (6-1), (6-2) cannot be lumped for $f(x) \neq$ constant, the same proof cannot be applied to these problems. The most important equations for dx_1/dt which could be derived for this case are given in the following property:

Property 7:

If the optimal control policy $k^+(t)$ contains an unconstrained sub-policy S which is continuous, then

$$\frac{dx_1}{dt} = \frac{d}{dt} \int_0^1 p \lambda K F \psi dz \quad \text{on } S \tag{6-57}$$

and

$$\frac{dx_1}{dt} = \frac{1 - p}{p} \frac{d\bar{H}}{dt} \quad \text{on } S \tag{6-58}$$

Proof:

It has been shown by Crowe (1972) that at the optimum:

$$\frac{dx_1}{dt} = \frac{d}{dt} \int_0^1 (\mu k f g) dz \quad \text{for all } t \in [0,1] \tag{6-59}$$

Since from (6-14)

$$k \frac{\partial \bar{H}}{\partial k} = \int_0^1 (p \lambda K F \psi - \mu k f g) dz = 0 \quad \text{on } S \tag{6-60}$$

substituting (6-59) into (6-60) gives (6-57).

Similarly since from (6-13)

$$\frac{d\bar{H}}{dt} = \frac{d}{dt} \int_0^1 (\lambda K F \psi - \mu k f g) dz \tag{6-61}$$

Equation (6-58) follows directly by substituting (6-57) and (6-59) into (6-61). Q.E.D.

6.4 Numerical Results

In order to investigate the properties of the optimal inlet temperature policy for reactors where the catalyst decay is not a first-order reaction, a hypothetical reactor whose state equations are given by (6-1) and (6-2) with

$$F(x) = (1 - x)^n \tag{6-62}$$

$$f(x) = (1 - x)^r \tag{6-63}$$

and

$$g(\psi) = \psi^m \tag{6-64}$$

with $m \neq 1$, has been studied for various parameter settings.

A selection of problems with various combinations of the parameters p, n, r and m is given in Table 6-1. Different forms of the function f(x) have also been considered and are shown in Table 6-1.

The common parameters used in problems A1-A10 (unless otherwise mentioned in Table 6-1) were chosen as follows:

i) $x_o(t) = 0$ for all $t \in [o,1]$ (6-65)

ii) The catalyst deactivation energy

$$E_c/R = 15000°K \tag{6-66}$$

iii) The average space time for the reactor

$$t_\theta = 1 \text{ sec} \tag{6-67}$$

iv) The total operating time

$$t_f = \begin{cases} 25 \text{ days in case } m > 1 \\ 12.5 \text{ days in case } m < 1 \end{cases} \tag{6-68}$$

v) Upper and lower bounds on the admissible inlet temperature:

$$T^* = 900°K$$
$$T_* = 700°K \qquad (6\text{-}69)$$

vi) The pre-exponential constant in the Arrhenius expression for k[T]

$$k_o = 20.2447\ t_f \qquad (6\text{-}70)$$

except for problems A2 and A10 where $k_o = 20.24\ t_f$.

vii) The pre-exponential factor K_o in the Arrhenius expression for K[T] was calculated in such a way that:

1) for the given parameter settings of the problem
2) $x_o = 0$
3) $\psi(z) = 1$ for all $z \in [o,1]$
4) $T = T^*$

the exit conversion out of the reactor was $x_1 = 0.9$. The only exception to this problem A10 where K_o was determined as $K_o = -\ln(0.1)/\exp(-8750/1090)$.

The initial relative catalyst activity distribution $\psi_o(z)$ for the problems A1, A2, A7, A9 and A10 was

$$\psi_o(z) = 1 \quad \text{for all } z \in [o,1] \qquad (6\text{-}71)$$

However, since some of these calculations were done in conjunction with the numerical work which will be discussed in the next chapter,

the reactor system set-up was slightly different for problems A3-A6 and A8. For these problems, we considered two batches of catalyst, both of the same type but with different initial activity: ψ_{10} and ψ_{20} respectively. The catalyst load which was put in the reactor at initial time was considered to be a uniform mixture of equal amounts of the two catalysts. The only difference between this set-up and a reactor with only one catalyst uniformly distributed along the axis of the reactor at time zero and with an initial relative activity $\psi_0 = (\psi_{10} + \psi_{20})/2$, is that for a decay rate of order $m \neq 1$, the average relative catalyst activity in the reactor at time t' ; $0 < t' \leq 1$, would be different for both cases.

Although this system will be dealt with more in detail in the next chapter, it is clear that we now need to describe the catalyst decay by two expressions:

$$\psi_{it} = - k\, f(x) g(\psi_i) \qquad i = 1,2 \tag{6-72}$$

one for each of the two catalysts. Both expressions are similar but the initial conditions to each of them are respectively:

$$\begin{aligned} \psi_1(o,z) &= \psi_{10} \quad \text{for all } z \in [o,1] \\ \psi_2(o,z) &= \psi_{20} \quad \text{for all } z \in [o,1] \end{aligned} \tag{6-73}$$

The variable ψ in Equation (6-1) then simply can be replaced by $(\psi_1 + \psi_2)/2$. The values which were used for ψ_{10} and ψ_{20} in the calculations are given in Table 6-1. It is clear that $\psi_{10} = \psi_{20} = 1$ refers to an initial uniform

catalyst activity distribution as given in (6-71).

Whereas in problems A1-A9, the temperature inside the reactor was considered uniform, problem A10 represents a reactor under adiabatic operating conditions.

The parameter J' given in Table 6-1 is defined in Equation A-9 in Appendix A. The conversion dependent functions $\bar{F}(x)$ and $\bar{f}(x)$, defined in Appendix A by (A-13) and (A-15) respectively, can for the given parameter settings of problem A10 be written as:

$$\bar{F}(x) = (1 - x) \exp(7\, x/6.48) \qquad (6\text{-}74)$$

and

$$\bar{f}(x) = (1 + x) \exp(7\, x/3.24) \qquad (6\text{-}75)$$

We must mention however, that for the problem A10, the upper inlet temperature constraint has been kept constant, and therefore does not really correspond to a realistic adiabatic reactor. The upper constraint should in fact be determined by the highest temperature in the reactor and the reason why this has not been done is that we wanted to compare our results for this case with those obtained earlier by Jutan (1973) for the same problem.

6.4.1 Numerical Procedure and Results

Since for the quasi-steady state equations (6-1) and (6-2), the characteristic lines for the partial differential equations are orthogonal and parallel to the coordinate axes, the numerical procedure which was

used to calculate the optimal inlet temperature profile for each problem is identical to the procedure which has been described in Chapter 4 for the study of Problem Π_0.

The optimal inlet temperature policies and the corresponding exit conversion profiles which have been calculated for the problems A1-A10 are shown in Figures (6-2)-(6-11).

The relative improvements in the objective function for the calculated optimal inlet temperature policies over the best calculated constant inlet temperature performance for problems A1-A10 are summarized in Table 6-2.

6.4.2 Discussion

It is obvious from the Figures (6-2)-(6-11) that only those problems whose optimal control policy is partly unconstrained have been selected for this study. For many different combinations of the parameters, the optimal control policy was found to be totally constrained: $k^+(t) = k^*$ for all $t \in [0,1]$. Although an optimal bang-bang control type policy is feasible in this type of optimal control problems, none has been encountered during the numerical work of this study and no attempt has been made to find a problem of this type where the optimal control would be bang-bang.

From Table 6-1 we also notice that the value of the parameter p in the problems A1-A10 was chosen to be less than 1. Although it was shown in Property 4 that a partly unconstrained policy is a feasible control for optimality, problems which exhibit an optimal control which

Table 6-1: Various parameter settings for problems A1-A10

Problem	$p = E_R/E_c$	$F = (1-x)^n$ n	$f = (1-x)^r$ r	$g = \psi^m$ m	$\psi_o(z)$		t_f days	Comments
					ψ_{10}	ψ_{20}		
A1	.4	1.0	1.0	2.0	1.0	1.0	25	
A2	.2	1.0	1.0	2.0	1.0	1.0	25	$k_o = 20.24\ t_f$
A3	.5	1.0	1.0	.5	1.2	.8	12.5	
A4	.5	1.0	1.0	2.0	1.2	.8	25	
A5	.5	1.0	.5	.5	1.0	.6	12.5	
A6	.5	1.0	.5	2.0	1.0	.6	25	
A7	.5	2.0	.5	.5	1.0	1.0	12.5	
A8	.5	1.0	$f = x^2$	.5	1.0	.6	12.5	
A9	.5	2.0	$f = \frac{(1-x)^{.5}}{x}$	2.0	1.0	1.0	25	$x_o(t) = 0.1$
A10	.5	1.0	$f = 1 + x$	2.0	1.0	1.0	25	Adiabatic $J = -1/8100$ $E_c/R = 17500°K$ $T^* = 1000°K$

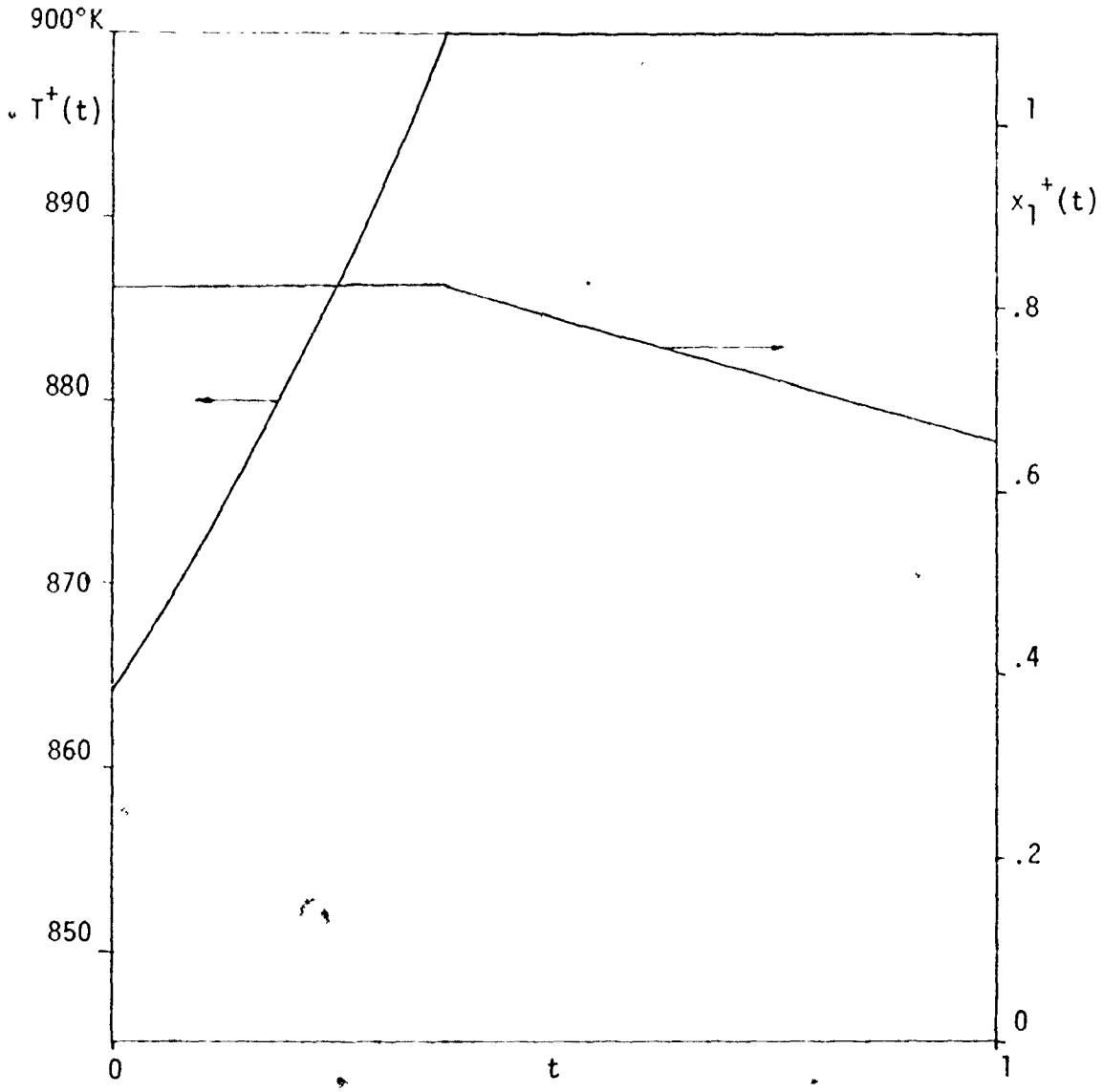

Figure 6-2: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A1.

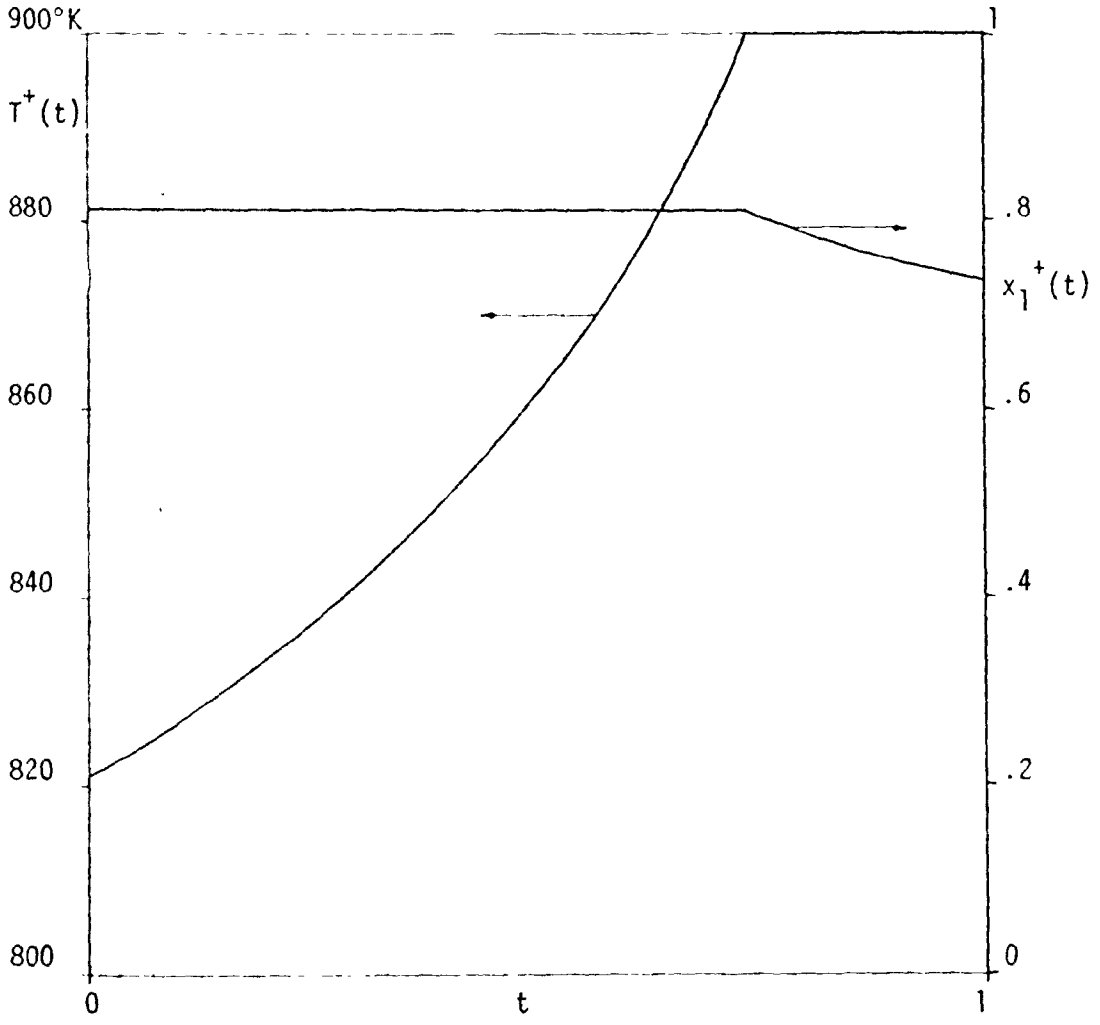

Figure 6-3: Optimal control policy $T^{+}(t)$ and exit conversion $x_1^{+}(t)$ for Problem A2.

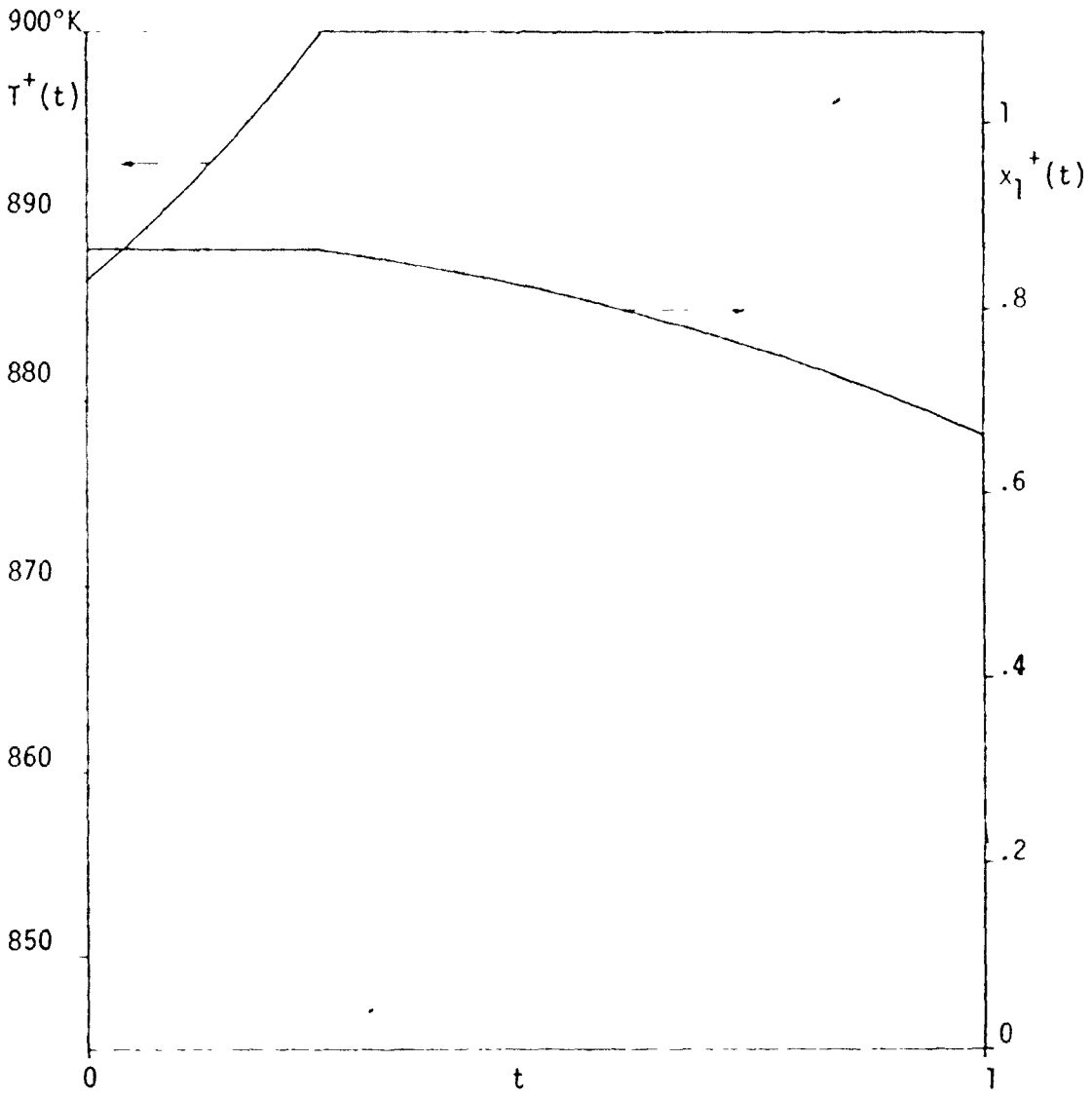

Figure 6-4: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A3.

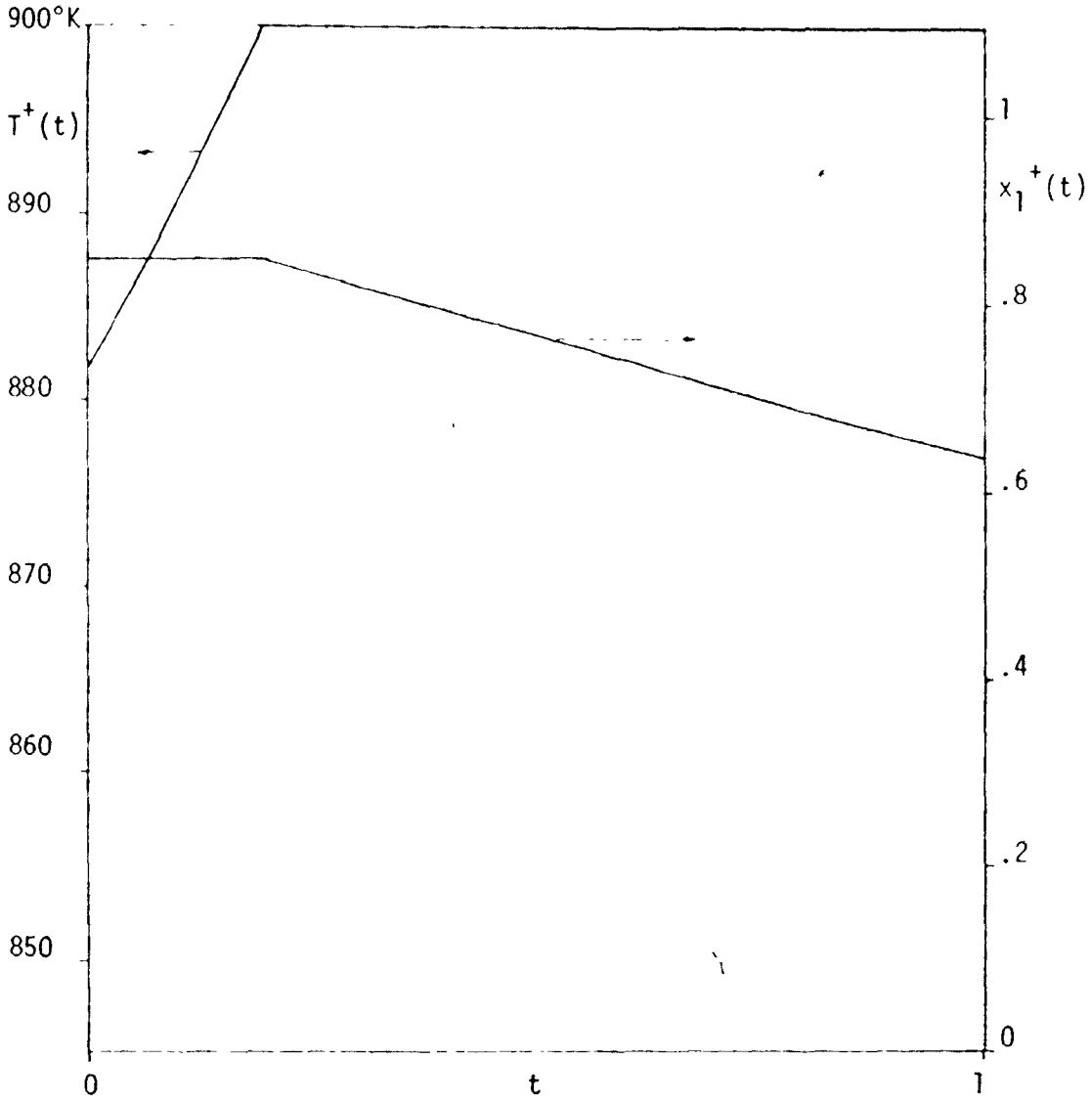

Figure 6-5: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A4.

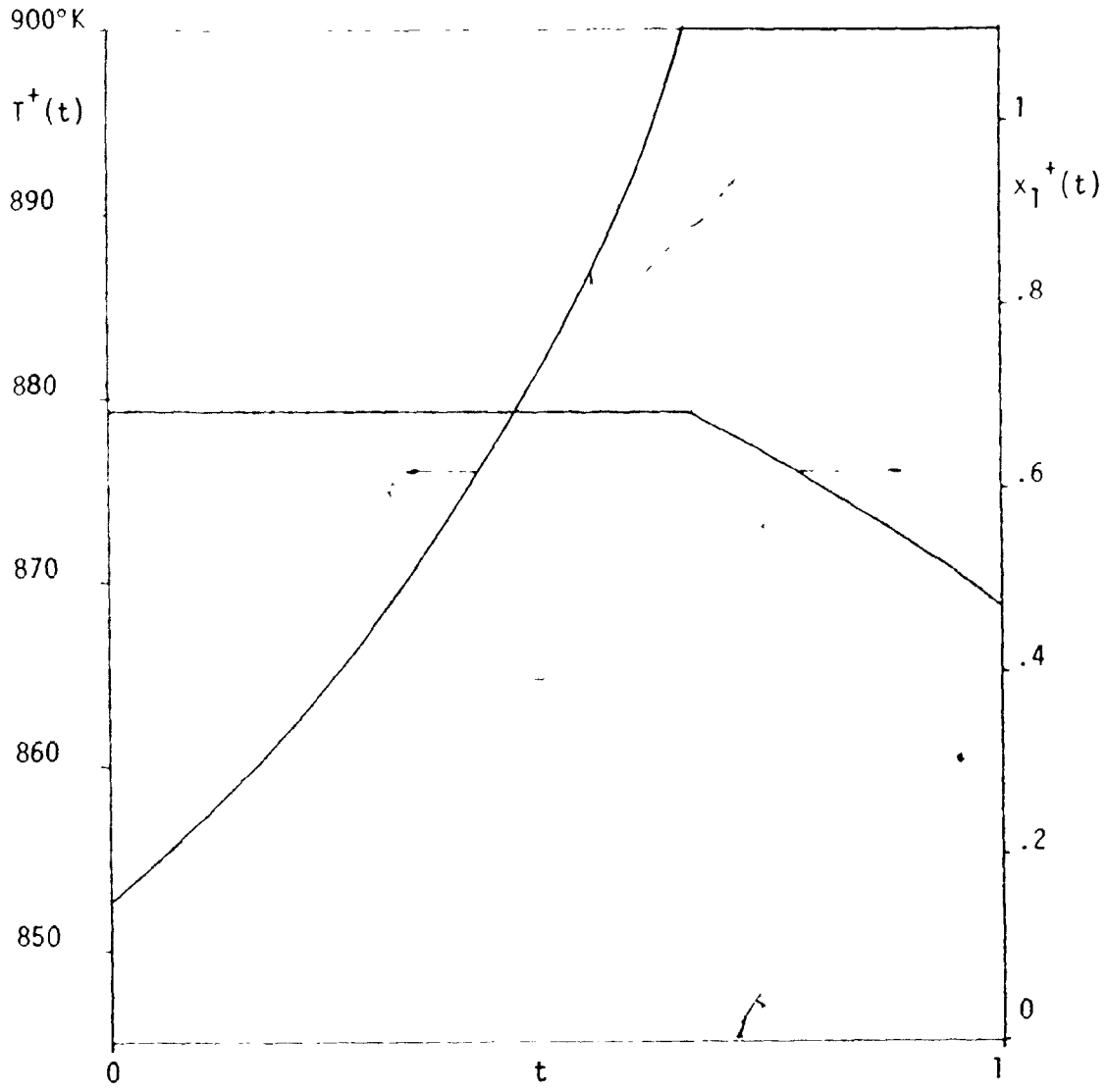

Figure 6-6: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A5.

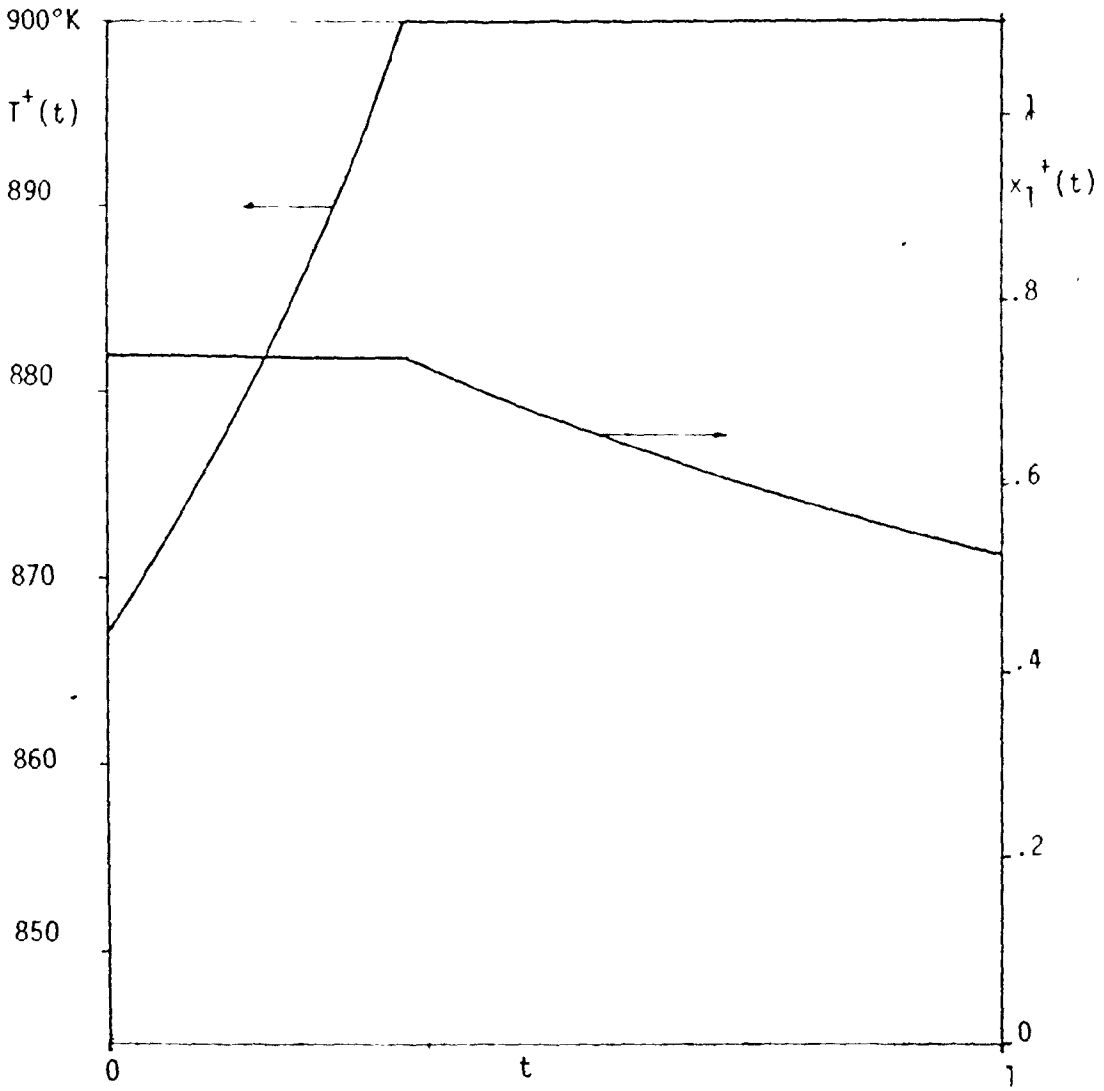

Figure 6-7: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A6.

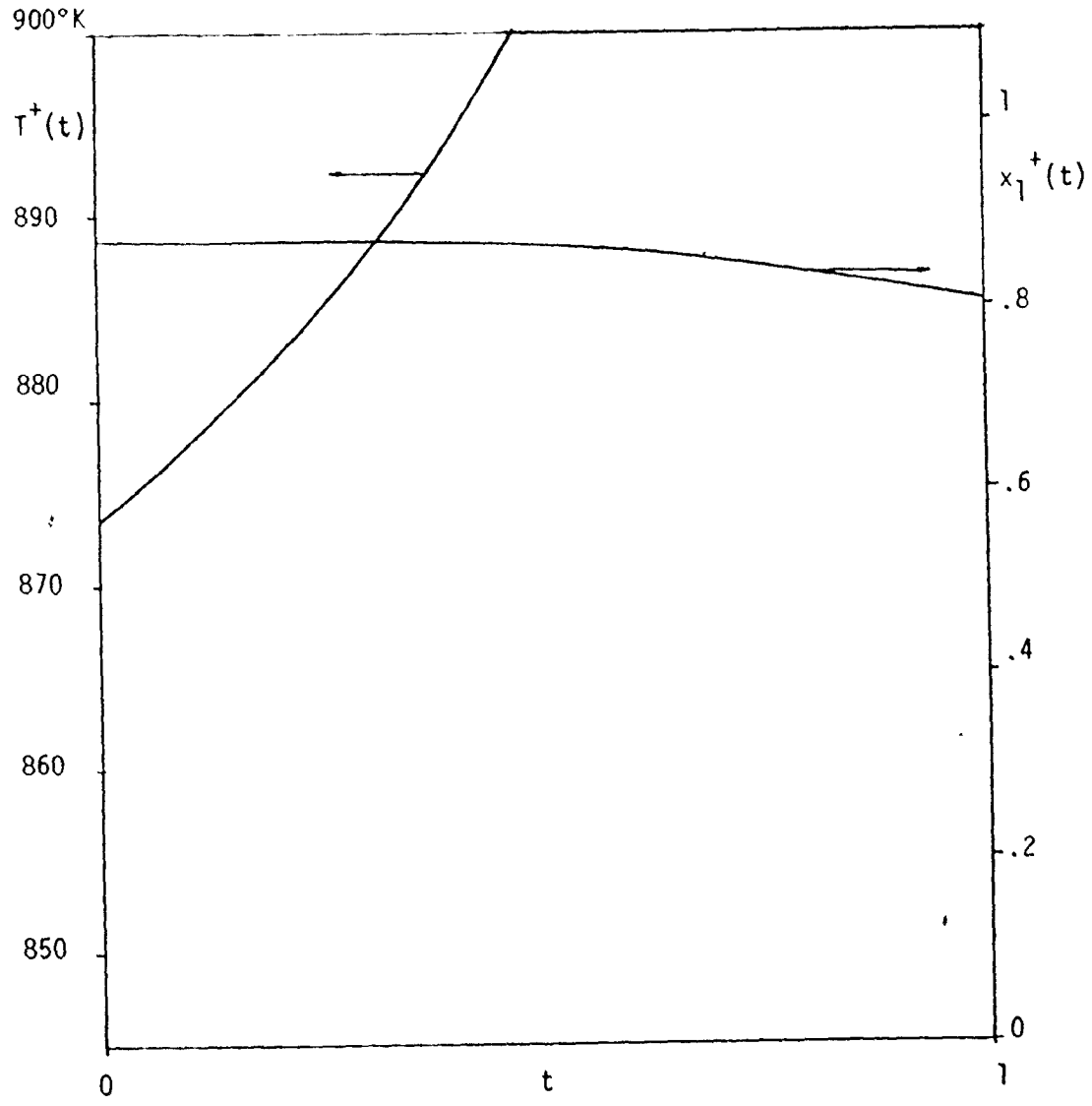

Figure 6-8: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A7.

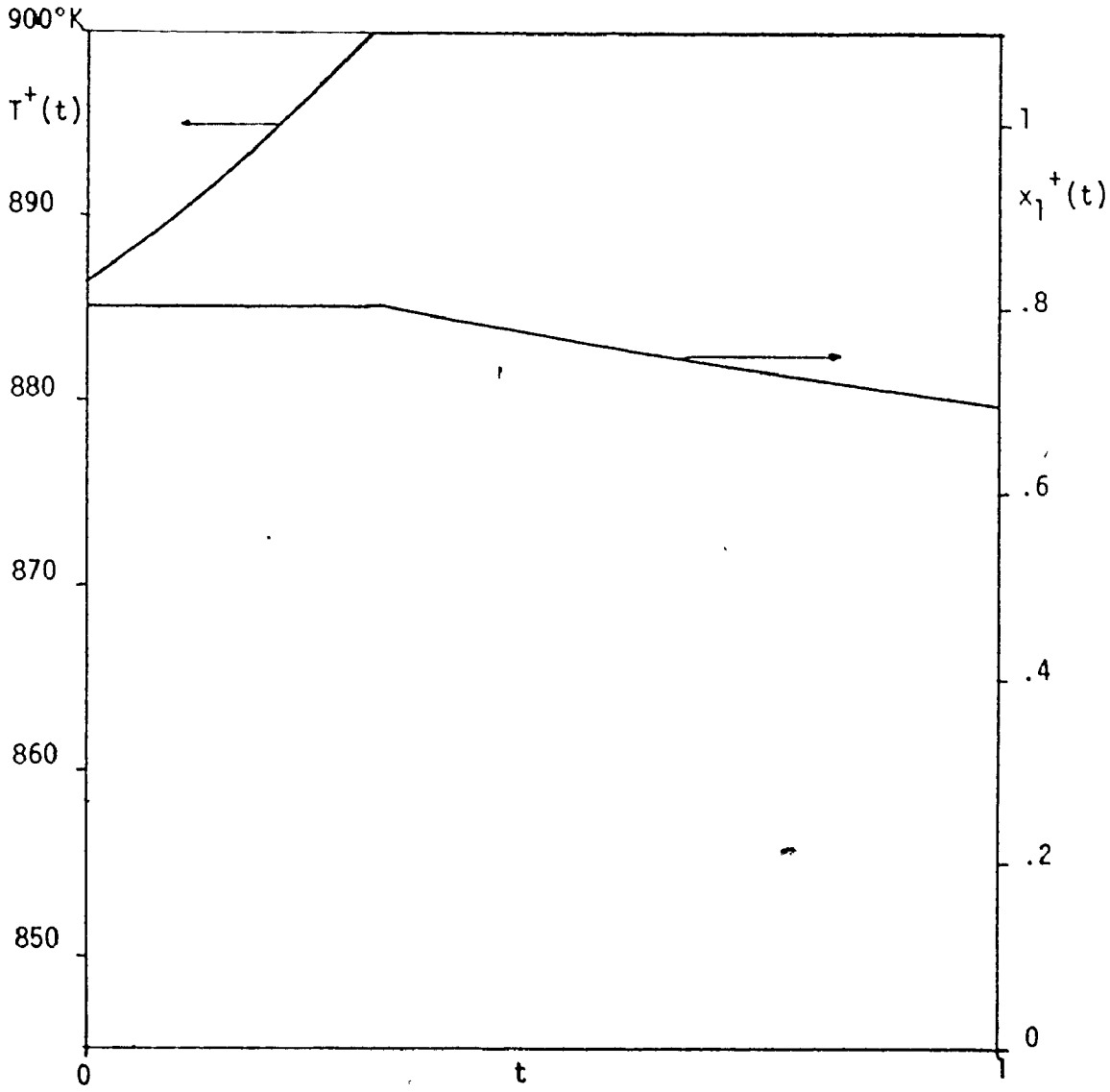

Figure 6-9: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A8.

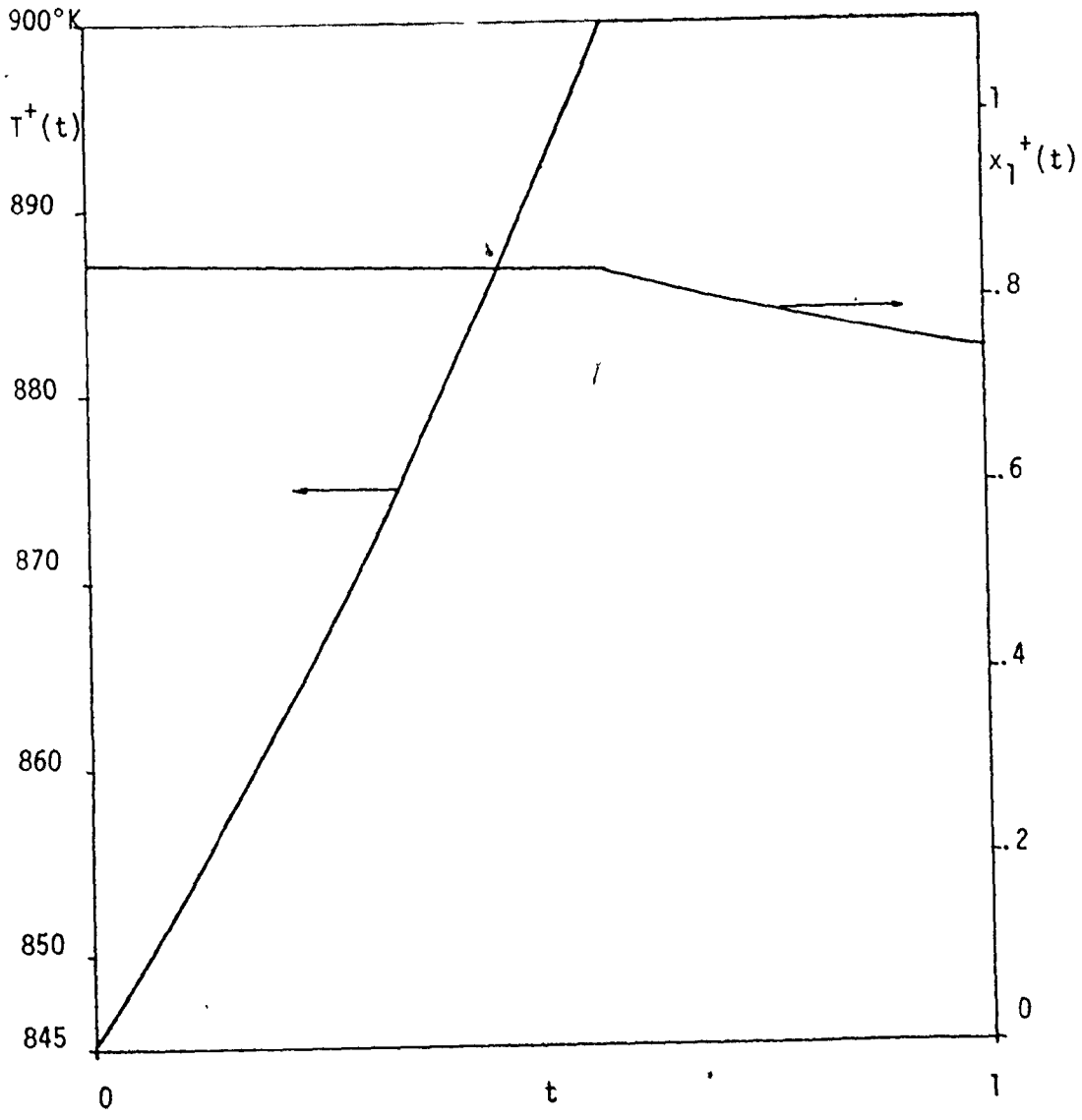

Figure 6-10: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A9.

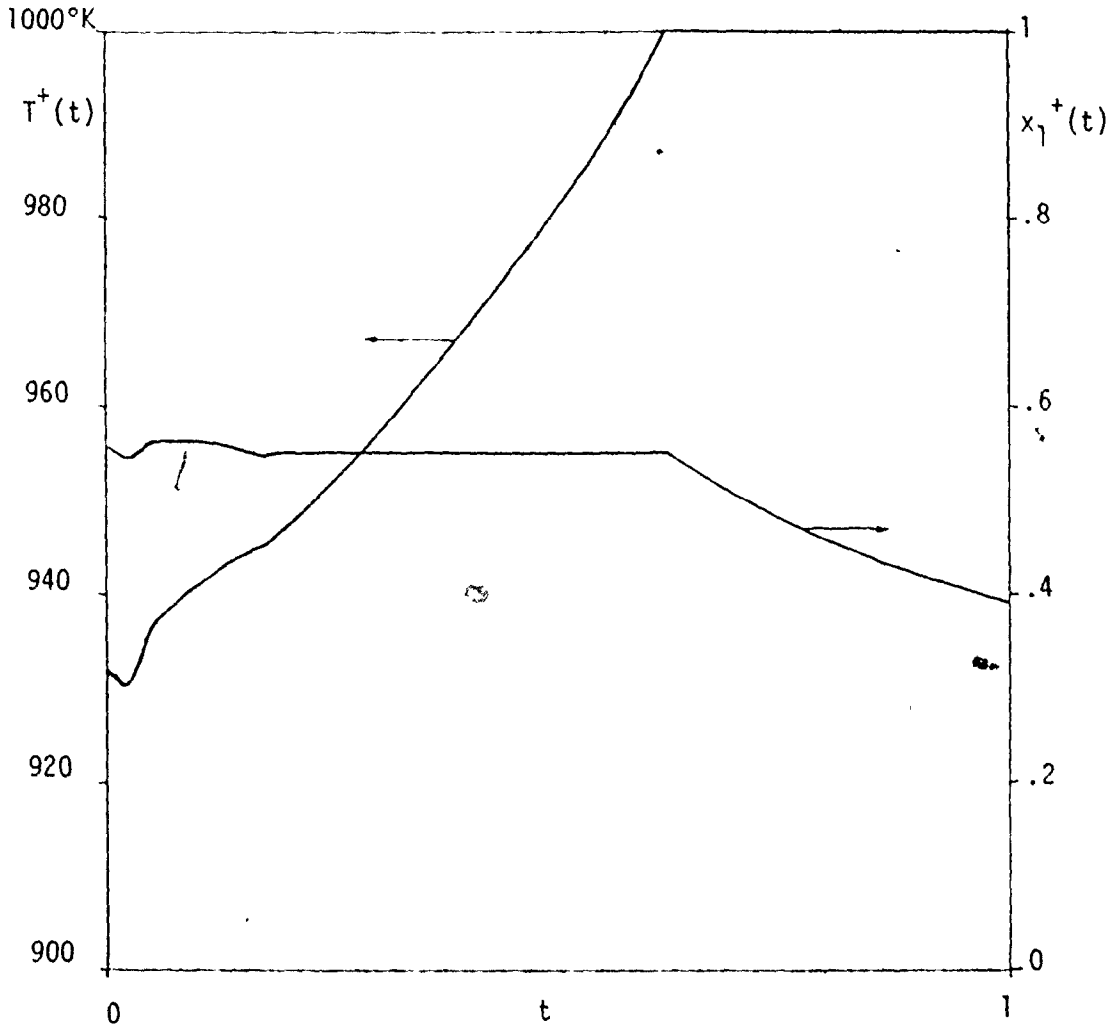

Figure 6-11: Optimal control policy $T^+(t)$ and exit conversion $x_1^+(t)$ for Problem A10.

Table 6-2: Relative improvement of the best boundary control policy $T^+(t)$ over the best constant inlet temperature policy for problems A1-A10.

Problem	Optimal policy p^+	Constant inlet temperature P_I	$\frac{P^+ - P_I}{P_I} \times 100\%$
A1	.7746935	.7710396	+ .474
A2	.8032328	.7883687	+1.885
A3	.8064748	.8059995	+ .059
A4	.7683645	.7678952	+ .061
A5	.6522725	.6344318	+2.812
A6	.6631000	.6591395	+ .601
A7	.8597998	.8578639	+ .226
A8	.7677564	.7667384	+ .133
A9	.7174310	.7089652	+1.194
A10	.5193415	.4789061	+8.443

is partly unconstrained for $p > 1$ are not very common. Such cases have been found, however, for certain combinations of the parameters and an example of such a problem was encountered as Problem Π_0 in Chapter 4.

Since in Table 6-1, usually more than one parameter has a different setting in any two problems, no conclusions will be drawn from these cases as to the effect of any of the parameters on the properties of the optimal control policy. Because of the fact that the constant exit conversion property has only been proven for conversion dependent decay problems where the order of decay m is equal to 1, the main motivation for the study of problems A1-A10, where $m \neq 1$, was to investigate the properties of the optimal exit conversion profile over the time interval where the optimal control was unconstrained.

The main conclusion which upon observation of the optimal exit conversion profiles in Figures (6-2) - (6-11) can be drawn is of course that the exit conversion at the optimum has been found to be constant over the time interval where the control is unconstrained in any one of the problems A1-A10.

Although many more calculations have been done for similar problems with different values of the parameters and $m \neq 1$, up to this date, no example has been found where the constant exit conversion property did not seem to hold. In the work done earlier by Jutan (1973), it was also found that for many problems of the type studied here, the optimal inlet temperature policy gave rise to the constant exit conversion property. Although the author also reported some calculated optimal policies which did not exhibit this property, it is believed that for those problems, the

computations were halted before convergence towards the optimal policy was achieved. Most of the problems where this was the case, have been recalculated and we found that besides the fact that we could increase the values of the objective functions found earlier, the corresponding optimal policies also all resulted in a constant exit conversion over the time interval where the optimal control was unconstrained. Our problems A1 and A10 are examples of this.

The main importance of a constant exit conversion property is that the optimal control policy can be determined from a one dimensional search on the inlet temperature at time zero. Once $T(o)$ has been specified, the total control policy $T(t)$ can then be calculated by calculating $T(t')$ for all $t' > 0$ such that $x_1(t) = x_1(o)$ for all $t \in [o,t']$. If at some point in time t_1, $T(t_1)$ reaches the upper constraint T^*, the control is then kept on that constraint until the end of the operation. The optimal control policy can be found as the one for which the objective function reaches a maximum with respect to $T(o)$. Remark that in this class of problems the optimal control could also consist of an initial finite time interval $[o,t_1) \subset [o,1]$ where the control is at its lower bound. In this case, the point in time t_1 where the control leaves the lower constraint, then determines the total policy. This for instance would happen whenever $T_* > T^+(o)$.

The constant exit conversion property is also important from the viewpoint of practical control implementation in that the value of the optimal constant exit conversion could be used as a setpoint.

The slight oscillation which is shown in the profiles for problem

A10 is due to the fact that the computer program was halted before total convergence to the stationary policy was reached. The gradient method which was used in updating the control policies usually converged in less than 10 iterations to a solution for which no further improvement in the value of the objective function was noticeable. The value of the partial derivative of the boundary hamiltonian with respect to the control over the unconstrained region was of the order of 10^{-5} at the optimum. The convergence for problem A10 however, was slower and the calculated profiles could still be improved. A conjugate gradient method for instance, could give better results in this case.

6.5 Unsteady State vs. Quasi-Steady State Formulation

The main difference in using the unsteady state expression (5-22) rather than the quasi-steady state equation (5-23) in the formulation of the optimal control problem is that the conversion characteristic in the unsteady state formulation is no longer parallel to the control characteristic, but forms, for small values of (t_θ/t_f), an angle of order (t_θ/t_f) radians with the lines along which the control remains uniform.

As has been shown in Chapter 4, this could possibly have the effect that although an optimal piecewise continuous controller exists for the quasi-steady state problem, there does not exist an optimal controller in this class of admissible control functions for the unsteady state problem.

Since an optimal pure relaxed controller is not physically realizable, sub-optimal control policies will have to be considered for practical

implementation. A sub-policy to the optimal relaxed control policy which chatters between two admissible control policies can for instance be chosen as a piecewise continuous control policy which switches a finite number of times between these two admissible policies. The frequency of switching then has an upper bound which can be determined from the physical limitations of such a control technique. This procedure also could be used in case the control characteristics are considered to have a steeper slope than the conversion characteristics. Since in a tubular fixed-bed reactor, the rate at which a change in temperature is carried through the reactor is smaller than the flowrate of the fluid stream, this latter representation of the control characteristics would be more realistic.

Other types of sub-optimal control policies which could be considered are the admissible control policy which was found to be optimal in the quasi-steady state system, or an admissible control policy which results in certain properties for the unsteady-state system which were found to be optimal in the quasi-steady state formulation, e.g., a control policy which gives a constant exit conversion out of the unsteady state reactor as long as the control variable is unconstrained.

A practical controller can then be chosen from among these sub-optimal policies.

CHAPTER 7

INITIAL CATALYST ACTIVITY DISTRIBUTION

7.1 Formulation of the Optimization Problem

For the boundary control problem where the distribution of the relative catalyst activity in the fixed-bed reactor at initial time is the control, the state equations for the reaction-deactivation system can be defined, similar to (6-1) and (6-2), as

$$x_z = K[T]\, F[x]\psi \tag{7-1}$$

and

$$\psi_t = -\, k[T]\, f[x]\psi^{\,m} \tag{7-2}$$

with the boundary condition

$$x(o,t) = x_o(t) \tag{7-3}$$

Since the inlet temperature is not a control variable, we specify the inlet temperature policy as

$$T(t) = T_o(t) \tag{7-4}$$

where $T_o(t)$ is a piecewise continuous function of t.

The boundary control variable is then the initial condition for the partial differential Equation (7-2)

$$\psi(z,o) = \psi_o(z) \tag{7-5}$$

where $\psi_o(z)$ will be sought in the class of piecewise continuous functions and is constrained by:

$$\psi_* \leq \psi_o(z) \leq \psi^* \quad \text{for all } z \in [o,1] \tag{7-6}$$

In addition to the constraint (7-6) we also will require that the average relative catalyst activity which is put in the reactor at time zero is constant:

$$\int_o^1 \psi_o(z)dz = c \tag{7-7}$$

The optimal control problem can then be written as

$$\max_{\psi_* \leq \psi_o(z) \leq \psi^*} P = \max_{\psi_* \leq \psi_o(z) \leq \psi^*} \int_o^1 [x_1(t) - x_o(t)]dt \tag{7-8}$$

subject to (7-1) - (7-4) and the constraint (7-7).

7.2 First-Order Deactivation Reaction: m = 1

As we have seen in Chapter 6, Section 6.3.1, when the order of deactiviation m is equal to 1, the state equations (7-1) and (7-2) can be formally integrated to give

$$x_1(t) = F(x_o(t),K\phi) \tag{7-9}$$

with

$$\frac{d\phi}{dt} = -\frac{k}{K}\, g(x_0(t), K\phi) \tag{7-10}$$

where

$$\phi(t) = \int_0^1 \psi(z,t)dz \tag{7-11}$$

With the inlet conversion and inlet temperature specified by (7-3) and (7-4), the exit conversion $x_1(t)$ given by (7-9) is for any $t \in [o,1]$ solely a function of the total integrated relative catalyst activity ϕ at that time.

From (7-10) it follows that with the inlet conditions specified, the integrated activity ϕ at any given time $t \in [o,1]$ can be calculated from the initial conditions of ϕ at time zero. However, since

$$\phi_o = \phi(o) = \int_0^1 \psi_o(z)dz \tag{7-12}$$

it follows from (7-7) that for any admissible initial distribution $\psi_o(z)$, the value of ϕ_o remains constant. This means that at any time $t \in [o,1]$ the value of $\phi(t)$ and hence $x_1(t)$ is totally determined from the inlet conditions (7-3), (7-4) and the value of ϕ_o. Hence for any initial distribution $\psi_o(z)$ which satisfies the constraint (7-7), the performance of the reactor will remain unchanged and therefore $\psi_o(z)$ cannot be considered as a boundary control variable.

7.3 Conversion Independent Decay and m ≠ 1

By letting f = 1 in (7-2), the relative catalyst activity at a point (z°,t°) in the z x t domain, for m ≠ 1, can be written as:

$$\psi(z^\circ,t^\circ) = [\psi_0(z^\circ)^q - q\int_0^{t^\circ} k(t)dt]^{1/q} \qquad (7\text{-}13)$$

where q = 1 - m.

For a uniform temperature reactor with T(t) specified by (7-4), we have

$$q\int_0^{t^\circ} k(t)dt = A(t^\circ) \qquad (7\text{-}14)$$

where A(t) is then a known function of t.

Substituting (7-13) and (7-14) in (7-1) and formally integrating gives

$$x_1(t^\circ) = F(x_0(t^\circ),\ K(t^\circ)\int_0^1 [\psi_0(z^\circ)^q - A(t^\circ)]^{1/q}dz^\circ) \qquad (7\text{-}15)$$

Since for m ≠ 1 and $t^\circ \in (0,1]$, the function $A(t^\circ)$ given by (7-14) is non-zero, Equation (7-15) shows that $x_1(t^\circ)$ cannot be expressed as a function of $\int_0^1 \psi_0(z)dz$. This would suggest of course that the exit conversion $x_1(t)$, and hence the value of the objective function, depends upon the distribution of the relative catalyst activity at initial time. From Equation (7-13) however, we see that for a uniform temperature reactor with f = 1, the relative catalyst activity at a point (z°,t°) in the z x t domain is totally determined by the initial activity $\psi_0(z^\circ)$ at

that point in the reactor and the temperature policy k(t) for t ϵ[o,t°]. This implies that for a given initial catalyst load with an initial catalyst activity distribution given by $\psi_o'(z)$, the performance of the reactor would be the same as for the case where the same initial catalyst load is distributed differently along the axis of the reactor to give an initial distribution $\psi_o''(z)$. Indeed, since the same catalyst is used to form both initial activity distributions, we would have that for any z^1 ϵ[o,1] there exists a z^2 ϵ[o,1] such that $\psi_o'(z^1) = \psi_o''(z^2)$. From (7-13) follows then that $\psi'(z^1) = \psi''(z^2)$ and hence the integrated relative activity $\phi(t)$ would be the same for both initial distributions for all t ϵ[o,1]. This would mean then that unless $\psi_o^+(z)$ = constant, the boundary control problem, in its present formulation, would give rise to an infinite number of solutions.

Since however, from (7-15) it follows that the exit conversion is not independent of the initial catalyst activity distribution, the optimal boundary control problem can be properly formulated as follows:

> "What is the optimal composition of a catalyst mixture placed in the reactor at initial time and which satisfies the constraint (7-7)?"

Rather than referring to the distribution of the catalyst along the axis of the reactor, this formulation allows us to consider problems where for instance a certain number of catalyst batches is available, all with different relative activities, but all of the same type. This situation can certainly be encountered in industrial processes where often besides fresh catalyst, batches of regenerated catalyst with lower

relative activities are available. The optimization problem would then become one of choosing either a catalyst load which consists of one batch of catalyst with uniform activity or a catalyst load which is composed of two or more batches of catalyst, each with different activity, but such that the total integrated relative activity of the initial load remains the same.

For the reaction-deactivation problem with $m \neq 1$ and the deactivation not dependent upon the conversion, certain characteristics of the choice of catalyst activities can now be derived.

Property 1:

> For $0 < m < 1$, the performance of the reactor with specified total initial catalyst activity is better for an initial catalyst load which is composed of two catalyst activities ψ_{10}, $\psi_{20} (\psi_{10} \neq \psi_{20})$, than for an initial load of catalyst with uniform activity ψ_{uo}.

Proof:

For given inlet conditions $x_0(t)$ and $T_1(t)$, it follows from (7-9) that the exit conversion at any time $t' \in [o,1]$ is only a function of the integrated relative activity ϕ at that time t'. Hence in order to prove the property it is sufficient to prove that for a mixture of catalyst activities, the integrated activity at any time $t' \in (o,1]$ is always larger than that obtained from an initial uniform activity load.

Let us consider a mixture of equal amounts of two batches of

catalyst with initial activity $\psi_{10} > 0$ and $\psi_{20} > 0$ respectively. Since the total initial activity is specified, we have to consider a catalyst load with uniform activity ψ_{uo} given by

$$\psi_{uo} = (\psi_{10} + \psi_{20})/2 \tag{7-16}$$

If two equal amounts of ψ_{10} and ψ_{20} are not used, the property still holds but the equations in the proof become more complicated.

Consider a point in time $t^\circ \in (o,1]$.

At t°, the catalysts with initial activities ψ_{10}, ψ_{20} and ψ_{uo} have decayed to ψ_1', ψ_2' and ψ_u' respectively and from (7-13) we can write

$$\psi_1' = [\psi_{10}^q - A']^{1/q} \tag{7-17}$$

$$\psi_2' = [\psi_{20}^q - A']^{1/q} \tag{7-18}$$

$$\psi_u' = [\psi_{uo}^q - A']^{1/q} \tag{7-19}$$

where $q = 1 - m$

and

$$A' = q \int_o^{t^\circ} k(t)dt$$

Since $0 < m < 1$, we have $0 < q < 1$ and $A' > 0$. We also assume that the total operating time is such that the catalyst activities remain positive at the final time.

Hence we now need to prove that for any $t^\circ > 0$

$$(\psi_1' + \psi_2')/2 \rightarrow \psi_u' \tag{7-20}$$

or from (7-17) - (7-19) and (7-16)

$$([\psi_{10}^q - A']^{1/q} + [\psi_{20}^q - A']^{1/q})/2 > \{[(\psi_{10} + \psi_{20})/2]^q - A'\}^{1/q} \tag{7-21}$$

for all $0 < q < 1$ and all $A' > 0$.

Although the proof can be totally constructed in an analytical fashion, it is easier and more illustrative to make use of geometrical arguments.

In Figure (7-1), a graph of the function ψ^q vs. ψ has been represented. Since $0 < q < 1$, the curve is concave. The points representing ψ_1', ψ_2' and ψ_u' have been constructed from ψ_{10}, ψ_{20} and ψ_{uo} according to the Equations (7-17)-(7-19).

Through the relationship of ψ^q vs ψ, it is possible to eliminate ψ_{20} and ψ_2' from the equations as follows:

$$\psi_{20} = [\psi_{10}^q + d]^{1/q} \tag{7-22}$$

$$\psi_2' = [(\psi_1')^q + d]^{1/q} \tag{7-23}$$

We now define the following function:

$$L = \left(\frac{\psi + (\psi^q + d)^{1/q}}{2}\right)^q - \frac{\psi^q + (\psi^q + d)}{2} \tag{7-24}$$

The function L represents a line segment in the graph in Figure (7-1) bounded between the curve representing ψ^q and a chord to this curve. The segments L_o and L' corresponding to ψ_{10} and ψ_1' are illustrated in

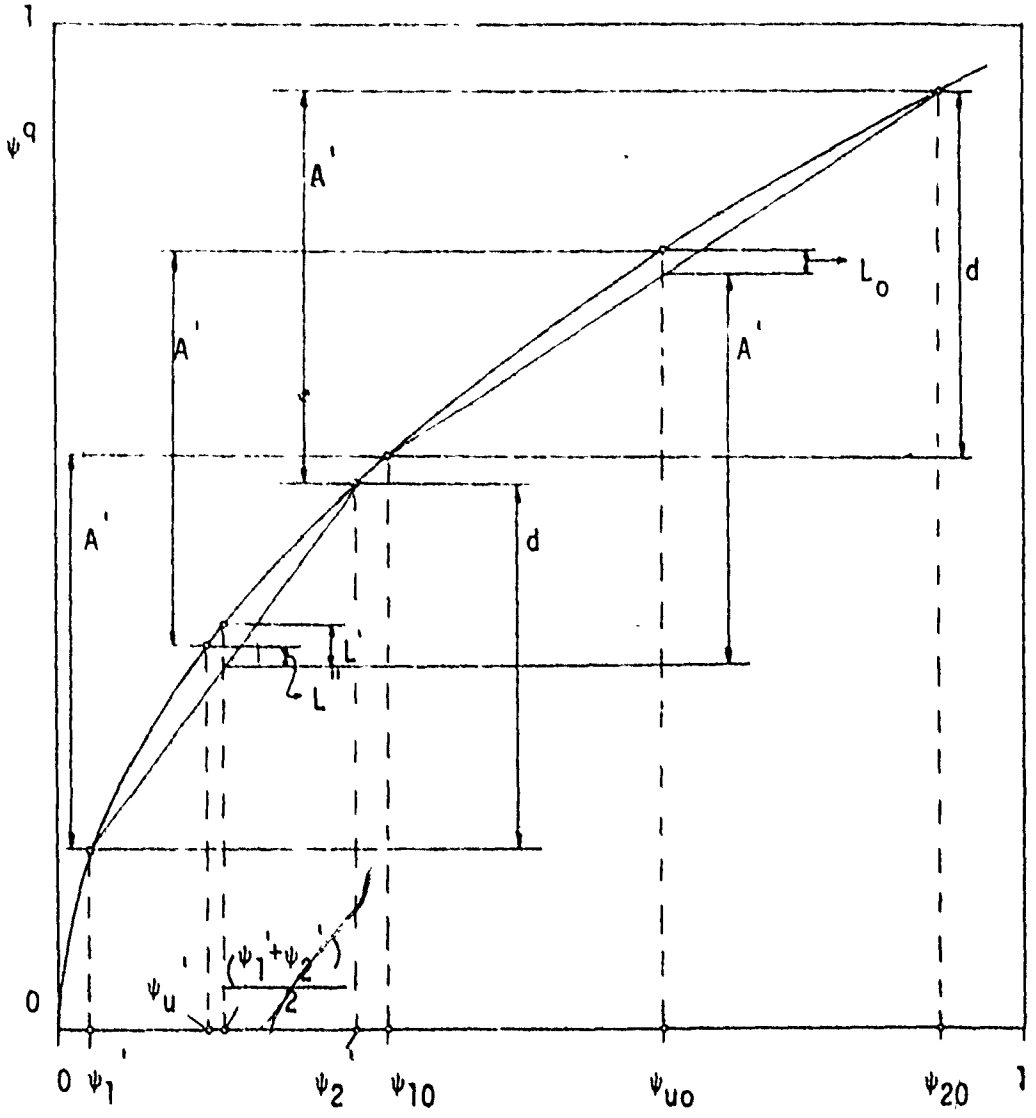

Figure 7-1: Graphical construction for proof of Property 1 with $q = .5$, $\psi_{10} = .36$, $\psi_{20} = .96$, $A' = .41$.

Figure (7-1).

In order now to prove the inequality (7-20) it can be seen from the graph in Figure (7-1) that it is sufficient to prove that $L' > L''$. From the geometry of the construction in the graph however, it is clear that $L'' = L_o$ and hence all we need to prove is that $L' > L_o$.

This now can easily be done from (7-24) as follows:

$$\frac{\partial L}{\partial \psi} = \frac{q}{2}\left(\frac{\psi + (\psi^q + d)^{1/q}}{2}\right)^{q-1}\left(1 + (\psi^q + d)^{(1-q)/q}\psi^{q-1}\right) - q\,\psi^{q-1} \qquad (7\text{-}25)$$

Since we assumed $\psi > 0$, this can be rearranged as follows:

$$\frac{\partial L}{\partial \psi} = q\,\psi^{q-1}\left(\frac{\psi + Y}{2}\right)^{q-1}\left[\frac{\psi^{1-q} + Y^{1-q}}{2} - \left(\frac{\psi + Y}{2}\right)^{1-q}\right] \qquad (7\text{-}26)$$

where

$$Y = (\psi^q + d)^{1/q} \qquad (7\text{-}27)$$

Now since $0 < 1 - q < 1$ for $0 < q < 1$, it follows from the concavity of the function ψ^{1-q} that for $\psi > 0$ and $Y > 0$ the expression in the square brackets in Equation (7-26) is negative.

Thus:

$$\frac{\partial L}{\partial \psi} < 0 \qquad (7\text{-}28)$$

and since $\psi_1' < \psi_{10}$, this implies that $L' > L_o$ in Figure (7-1). Q.E.D.

The proof of (7-20) for the case where $\psi_{10} = 0$ is much simpler and follows directly by substituting (7-16), (7-18) and (7-19) into (7-20)

noting that $\psi_{10} = 0$ implies $\psi_1 = 0$. This latter case where $\psi_{10} = 0$ corresponds to diluting the catalyst with an inert material.

Property 2:

> For $m > 1$, the performance of the reactor with specified total initial catalyst activity is better for an initial catalyst load which has a uniform relative activity ψ_{uo} than for a mixture of two catalysts with initial activities ψ_{10} and ψ_{20} $(\psi_{10} \neq \psi_{20})$.

Proof:

The proof of this property follows the same steps as in the proof of Property 1, but since the function ψ^q is convex for $q = 1 - m < 0$, the opposite conclusion is reached.

7.4 Conversion Dependent Decay and $m \neq 1$

Although for this problem the distribution of the initial catalyst activity becomes a control variable, we will limit the analysis of this problem to the case where we have two catalysts of the same type, but with different initial activities, available. This is indeed a more realistic problem than trying to find the optimal control policy in terms of $\psi_0(z)$.

We will consider a mixture of equal amounts of catalyst with initial activities ψ_{10} and ψ_{20} respectively. The control variable then becomes the concentration of both catalysts in the mixture which is put

into the reactor. By defining this control variable as a(z), we have the effective relative catalyst activity at a point z° e[o,1] in the reactor at a time t° e[o,1] then given by

$$\psi_{eff}(z°,t°) = a(z°)\ \psi_1(t°) + (1 - a(z°))\ \psi_2(t°) \qquad (7\text{-}29)$$

where $\psi_1(t°)$ and $\psi_2(t°)$ are the activities of the respective catalysts at time t°.

Since the catalyst at each point z° e[o,1] inside the reactor is a mixture of two catalysts with different activities, we need a decay rate expression for each of the two catalysts. Substituting (7-29) for ψ in (7-1), the state equation then can be written as

$$x_z = K\ F(a\psi_1 + (1\text{-}a)\ \psi_2) \qquad (7\text{-}30)$$

$$\psi_{1t} = -\ kfg_1 \qquad (7\text{-}31)$$

$$\psi_{2t} = -\ kfg_2 \qquad (7\text{-}32)$$

where $g_i = \psi_i^m$, $\quad i = 1,2.$

The initial and boundary conditions for (7-30) - (7-32) are

$$x(o,t) = x_0(t) \qquad (7\text{-}33)$$

$$T(o,t) = T_0(t) \qquad (7\text{-}34)$$

$$\psi_1(z,o) = \psi_{10} \quad \text{for all } z \in [o,1] \qquad (7\text{-}35)$$

$$\psi_2(z,o) = \psi_{20} \quad \text{for all } z \in [o,1] \qquad (7\text{-}36)$$

The control variable a(z) is constrained by

$$0 \leq a(z) \leq 1 \tag{7-37}$$

and the total initial catalyst activity is specified as

$$\int_0^1 [a(z)\ \psi_{10} + (1-a(z))\ \psi_{20}]dz = c \tag{7-38}$$

or since it is specified that equal amounts of both catalysts are used, Equation (7-38) can be written as

$$\int_0^1 a(z)dz = 0.5 \tag{7-39}$$

The optimal control problem then can be written as

$$\max_{0 \leq a(z) \leq 1} P = \max_{0 \leq a(z) \leq 1} \int_0^1 [x_1(t) - x_0(t)]dt \tag{7-40}$$

where a(z) is sought in the class of piecewise continuous controls and has to satisfy the constraint (7-39).

7.4.1 Necessary Conditions for Optimality

Application of the maximum principle technique for boundary control then leads to the hamiltonian

$$H = \lambda\ K\ F(a\psi_1 + (1-a)\ \psi_2) - \mu_1 kfg_1 - \mu_2 kfg_2 \tag{7-41}$$

where the adjoint variables λ, μ_1 and μ_2 are solutions of

$$\lambda_z = -\frac{\partial H}{\partial x} \tag{7-42}$$

$$\mu_{1t} = -\frac{\partial H}{\partial \psi_1} \tag{7-43}$$

$$\mu_{2t} = -\frac{\partial H}{\partial \psi_2} \tag{7-44}$$

with

$$\lambda(1,t) = 1 \quad \text{for all } t \in [0,1] \tag{7-45}$$

$$\mu_1(z,1) = \mu_2(z,1) = 0 \quad \text{for all } z \in [0,1] \tag{7-46}$$

Since the control $a(z)$ is a function of z only and since any admissible control policy also has to satisfy the constraint (7-39), the boundary hamiltonian $\bar{H}$ is defined as

$$\bar{H} = \int_0^1 H\, dt - \kappa\left(\int_0^1 a(z)dz - .5\right) \tag{7-47}$$

where κ is a constant Lagrange multiplier. This boundary hamiltonian is different from the forms discussed in Chapter 3 in that it contains an additional term which takes care of the constraint (7-39). This form of the boundary hamiltonian can also be derived from a first-order perturbation analysis of the objective function.

The weak maximum principle for boundary control then requires the optimal control policy $a^+(z)$ to satisfy the following necessary conditions:

$$\frac{\partial \bar{H}}{\partial a} = \int_0^1 \lambda\ K\ F(\psi_1 - \psi_2)dt - \kappa \begin{cases} \geq 0 & \text{for } a^+(z) = 1 \quad (7\text{-}48) \\ \leq 0 & \text{for } a^+(z) = 0 \quad (7\text{-}49) \\ = 0 & \text{for } 0 < a^+(z) < 1 \quad (7\text{-}50) \end{cases}$$

Since $\partial \bar{H}/\partial a$ is not an explicit function of the control variable $a(z)$, the application of the maximum principle does not lend itself to determine any particular properties of the optimal control policy. A further difficulty is caused by the fact that the constant Lagrange multiplier κ is unknown. Although in general we can expect the optimal control to be bang-bang as determined by (7-48) and (7-49), we cannot exclude the possibility of having a singular control sub-policy, determined by (7-50) over all or part of the z-domain.

7.4.2 Numerical Procedure

Under the quasi-steady state assumptions, the state and adjoint equations (7-30) - (7-32) and (7-42) - (7-44) can again be integrated as ordinary differential equations along lines which are parallel to the coordinate axes.

For a given control policy $a(z)$, the integral

$$D \equiv \int_0^1 \lambda\ K\ F(\psi_1 - \psi_2)dt \qquad (7\text{-}51)$$

can be evaluated at each grid point along the z-axis.

If the chosen control $a(z)$ does not satisfy the necessary conditions (7-48) - (7-49), a new control policy can be determined as $a(z) + \delta a(z)$ where $\delta a(z)$ can be chosen as

$$\delta a(z) = \eta \left(\int_0^1 \lambda K F(\psi_1 - \psi_2) dt - \kappa \right) \tag{7-52}$$

with η a small positive parameter.

The new control policy has to satisfy the constraints (7-37), (7-39):

$$0 \leq a(z) + \delta a(z) \leq 1 \tag{7-53}$$

and

$$\int_0^1 [a(z) + \delta a(z)] dz = 0.5 \tag{7-54}$$

From (7-54) and (7-39) this last condition becomes:

$$\int_0^1 \delta a(z) dz = 0 \tag{7-55}$$

Since the conditions (7-48) - (7-50) apply for the optimal control policy, the value of κ is totally unknown as long as we do not know the optimal policy. Hence in order to calculate $\delta a(z)$ from (7-52), we have to make use of an approximation κ_1 for the value of .

Although it is easy to adjust a new control policy such that the constraints of (7-53) are satisfied, the condition (7-55) is a much more difficult one to comply with. Indeed, it is no longer sufficient to set $a(z) = 1$ (o) whenever $a(z) + \delta a(z) > 1$ (<o) since $\int_0^1 a(z) dz$ would no longer remain constant. This difficulty can be resolved by using appropriate values of κ_1 and η in the updating procedure.

Let us consider the z-axis divided into N equal intervals Δz and let us denote the discrete points along the z-axis in ascending order from 0 to N. We will consider the control to vary linearly between two adjacent grid points. Several possibilities for the control a(z) are now possible.

1) The control a(z) is totally unconstrained.

In this case we calculate κ_1 as follows:

$$\kappa_1 = \frac{\sum_{i=1}^{N} (D_{i-1} + D_i)}{2N} \tag{7-56}$$

where D_i is the value of the integral (7-51) at the i^{th} grid point along the z-axis. This value of κ_1 is then substituted for κ in (7-52). The value of η which is used in (7-52) is then chosen such that the constraint (7-53) is not violated.

2) The control a(z) is partly constrained.

Although several possibilities can occur here, we will illustrate the updating technique for two basic control adjustments. Consider for instance, a control policy a(z) which is initially constrained at a(z) = 1 and then remains unconstrained for the remainder part in the reactor. Let j denote the last discrete point where the control is constrained. (Figure 7-2a).

Case A: D_i is a decreasing function of i for i = j,...,N. In this case the control a(z) is updated to a(z) + δ a(z) only over the region where a(z) is unconstrained. By calculating κ_1 from the following equation:

$$(\kappa_1 + D_{j+1}) \frac{\Delta z}{2} + \sum_{i=j+2}^{N} (D_{i-1} + D_i) \frac{\Delta z}{2} = \kappa_1 (N - j)\Delta z \qquad (7\text{-}57)$$

we get

$$\kappa_1 = \frac{D_{j+1} + \sum_{i=j+2}^{N} (D_{i-1} + D_i)}{2(N - j - .5)} \qquad (7\text{-}58)$$

The derivation of Equation (7-57) can easily be seen from Figure 7-2b . By substituting κ_1 for κ in (7-52), the control can then be updated at the points j+1 to N and it can easily be verified that by choosing κ_1 from (7-58), condition (7-55) will not be violated. The value chosen for η has to be such that also (7-53) is not violated.

Case B: D_i is an increasing function of i for i = j,...,N. In this case we allow the control a(z) to become unconstrained at the point j but keep the control at the constraint for the point j - 1. From Figure 7-2c we can derive the relationship

$$(\kappa_1 + D_j) \frac{\Delta z}{2} + \sum_{i=j+1}^{N} (D_{i-1} + D_i) \frac{\Delta z}{2} = \kappa_1 (N - (j-1))\Delta z \qquad (7\text{-}59)$$

and hence

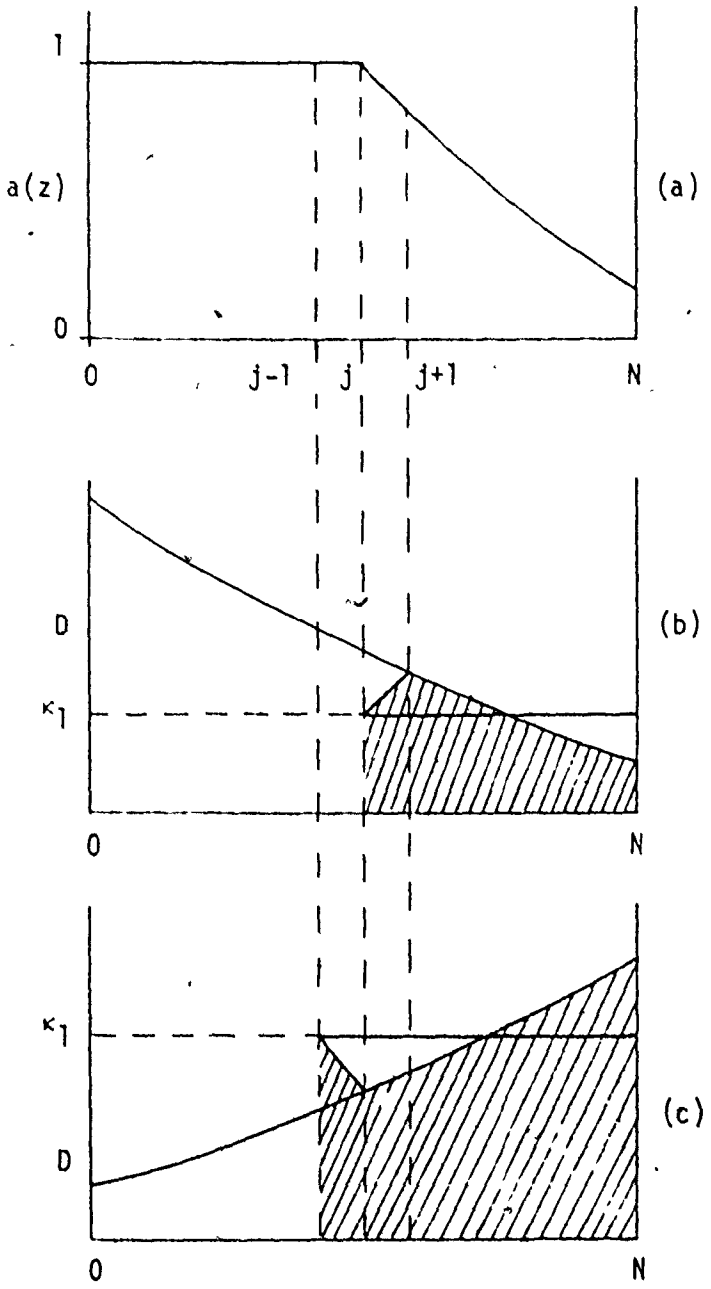

Figure 7-2: Illustration of the calculation of κ_1 used in updating the control a(z).

$$\kappa_1 = \frac{D_j + \sum_{i=j+1}^{N} (D_{i-1} + D_i)}{2(N - j + .5)} \qquad (7\text{-}60)$$

By updating the control now at the discrete points j to N, we can again verify that by substituting κ_1 from (7-60) into (7-52), the condition (7-55) is satisfied. The value of η again has to be chosen such that (7-53) is not violated.

A similar technique is used for the calculation of κ_1 when the control is at its lower constraint. For the more complex case where the control is on one of its constraints over more than one segment of the z-axis, the appropriate value of κ_1 can still be calculated in the same manner provided the same adjustments, as illustrated in Figure 7-2, are made whenever an unconstrained segment joins a constrained one. Although this method of adjusting the control could fail when D_i does not vary monotonically with respect to i, we have not encountered any such difficulties in our calculations. One of the possibilities which has to be taken into account for the numerical work is that the control $a^+(z)$ can be discontinuous. Using the updating technique described above, a discontinuous optimal control policy would be indicated by the fact that the region over which the control is unconstrained, becomes smaller and smaller during the iterations. Since however, discontinuities in the control a(z) are carried through along the lines which are parallel to the t-axis, this situation does not lead to serious difficulties in the integration, and can easily be incorporated in the algorithm.

7.4.3 Numerical Results and Discussion

The optimal initial distribution of a mixture of equal amounts of two catalysts along the axis of the reactor has been calculated for a number of problems with $m \neq 1$ and $f' \neq 0$.

The results which are presented here have been calculated for the problems with $F = 1 - x$ and all possible combinations of $f = x$, $f = 1 - x$, $m = .5$ and $m = 2$. The common parameters in these problems were identical to those discussed in Chapter 6, Section 6.4. The value of p was chosen as 0.5 and the inlet temperature policy was specified as:

$$T_0(t) = 900°K \quad \text{for all } t \in [0,1] \tag{7-61}$$

The initial catalyst activities for the two catalysts was chosen as

$$\psi_{10} = 1.2 \; ; \; \psi_{20} = .8 \tag{7-62}$$

The resulting optimal policies for the four combinations of the functions f and the values of m are tabulated in Table 7-1.

The values of the objective function P^+ corresponding to the optimal control policy $a^+(z)$ have been compared with those of P_{UM}, corresponding to a uniform mixture of the two catalyst ($a(z) = .5$ for all $z \in [0,1]$), and to the values of P_{UA}, corresponding to the same reactor system but with an initial uniform catalyst activity: $\psi_0 = (\psi_{10} + \psi_{20})/2 = 1$. The values of P^+, P_{UM} and P_{UA} for problems I-IV and the relative differences between P^+ and P_{UM} and between P^+

Table 7-1: Optimal control policies $a^+(z)$ for Problems I-IV.

Problem	f	m	Optimal Control Policy
I	x	2	$a^+(z) = \begin{cases} \Gamma & z \in [0,.5] \\ 0 & z \in (.5,1] \end{cases}$
II	x	.5	$a^+(z) = \begin{cases} 0 & z \in [0,.5] \\ 1 & z \in (.5,1] \end{cases}$
III	1-x	2	$a^+(z) = \begin{cases} 0 & z \in [0,.5] \\ 1 & z \in (.5,1] \end{cases}$
IV	1-x	.5	$a^+(z) = \begin{cases} 1 & z \in [0,.5] \\ 0 & z \in (.5,1] \end{cases}$

and P_{UA} are tabulated in Table 7-2.

From the observation of the results in Tables 7-1 and 7-2, the following conclusions can be drawn:

1) The optimal control is a bang-bang type control. Although a singular control policy is a feasible control for optimality, none has been encountered in our calculations.
2) The type of optimal bang-bang policy is determined by the sign of the product $(m - 1)f'$. If this sign is positive, the catalyst with the highest relative activity is placed in the first half of the reactor. If the sign is negative, the best catalyst is placed at the end. This would suggest that for industrial reactors where fresh catalyst is added to regenerated catalyst which has a lower relative activity, it would be advantageous to keep both catalysts separate in the reactor whenever the catalyst decay is conversion dependent and the decay rate is not of first-order.
3) A uniform mixture of two catalysts with different activities gives rise to a value of the objective function which is larger (smaller) than the one obtained from a reactor with a uniform catalyst activity, with the total integrated initial activity equal in both cases, when the order of deactivation m is smaller (greater) than 1. This has been proven in 7.3 for the case with conversion independent decay. Although the optimal distribution of the two catalysts for problems I and III in Table 7-2 is still better than an

initial catalyst load with uniform activity, we do not expect this always to be true for any of the parameter settings or for different functions F and f in the case of $m > 1$.

Table 7-2: Values of the objective function corresponding to the optimal control, a uniform catalyst mixture and a catalyst with uniform activity for problems I-IV.

Problem	P^+	P_{UM}	P_{UA}	$\frac{P^+-P_{UM}}{P_{UM}} \times 100\%$	$\frac{P^+-P_{UA}}{P_{UA}} \times 100\%$
I	.7638118	.7607095	.7629920	+ .408	+ .107
II	.7904205	.7860636	.7851064	+ .554	+ .677
III	.7727597	.7678952	.7710396	+ .633	+ .223
IV	.8114842	.8059995	.8049588	+ .680	+ .811

CHAPTER 8

INLET TEMPERATURE AND FLOW RATE CONTROL

8.1 Formulation of the Problem

In this section we will consider an optimal control problem with two boundary control variables: the inlet temperature and the inlet flow rate into the reactor. Assuming that there is no volumetric expansion inside the tubular reactor, the unsteady state reaction equation (5-23) with $t_0 = L/v$ can be written as

$$x_t + v(t_f/L)x_z = K F \psi \qquad (8\text{-}1)$$

where v is the linear flow rate, t_f the total operating time and L the length of the reactor bed.

Unless v(t) or k(t) vary too rapidly, the quasi-steady state approximation can often be used and (8-1) then can be written as

$$x_z = (L/t_f)K F \psi/v \qquad (8\text{-}2)$$

Since the value of (L/t_f) is constant for a problem with given final time, this factor can be absorbed into the rate constant K. Note, however, that by doing so, K is no longer dimensionless but has the units (length/time). Since the linear flow rate v(t) has the same units, the ratio K/v in the equation

$$x_z = \frac{K}{v} F \psi \tag{8-3}$$

is dimensionless. For the further discussion however, it is more convenient to work with dimensionless control variables. A dimensionless control variable for the linear flow rate can be obtained from:

$$v(t) = w(t)v_{av} \tag{8-4}$$

where w(t) is the control variable and v_{av} is the time average linear flow rate (i.e., $v_{av} = (\int_0^{t_f} v(t')dt')/t_f$). Since v_{av} will be kept constant, we can also absorb it in the rate constant K and we obtain

$$x_z = \frac{K}{w} F \psi \tag{8-5}$$

where now K and w are both made dimensionless. The catalyst deactivation equation remains unchanged and is given by

$$\psi_t = - kfg \tag{8-6}$$

Initial and boundary conditions to (8-5) and (8-6) are specified as

$$x(o,t) = x_o(t) \; ; \; \psi(z,o) = \psi_o(z) \tag{8-7}$$

Since the flow rate of the reactants can now vary with time, the total performance of the reactor can be measured by:

$$P_1 = \int_0^1 [x_1(t) - x_o(t)] \, w(t)dt \tag{8-8}$$

The boundary control variables k(t) and w(t) will be calllled admissible if they satisfy the following constraints:

$$k_* \leq k(t) \leq k^* \tag{8-9}$$

$$w_* \leq w(t) \leq w^* \tag{8-10}$$

and

$$\int_0^1 w(t)dt = 1 \tag{8-11}$$

This last constraint (8-11) implies from (8-4) that for a given total operating time, the total volume of reactants which has to be processed is fixed.

The optimal boundary control problem then consists of finding the piecewise continuous control functions $k^+(t)$ and $w^+(t)$ which satisfy the constraints (8-9) - (8-11) and for which P_1 is maximized over all admissible controls.

8.1.1 Application of the Maximum Principle

Although this particular form of the objective function (8-8) is not contained in the general objective function as given by (3-4), we still can employ the Equations (3-6) - (3-9) to define the hamiltonian function H as

$$H = \frac{\lambda K F \psi}{W} - \mu kfg \tag{8-12}$$

with the adjoint equations

$$\lambda_z = -\frac{\partial H}{\partial x} = -\frac{\lambda K F' \psi}{w} + \mu k f' g \tag{8-13}$$

$$\mu_t = -\frac{\partial H}{\partial \psi} = -\frac{\lambda K F}{w} + \mu k f g' \tag{8-14}$$

and

$$\lambda(1,t) = w(t) \; ; \; \mu(z,1) = 0 \tag{8-15}$$

From the first order perturbation analysis of the objective function P_1, as defined by (8-8), it is shown in Appendix B, that by using the Equations (8-12) - (8-15) the appropriate formulation of a boundary hamiltonian $\bar{H}$ then becomes

$$\bar{H} = \int_0^1 H dz + [x_1(t) - x_0(t)]\, w(t) - \kappa\left[\int_0^1 w(t)dt - 1\right] \tag{8-16}$$

where κ is a constant Lagrange multiplier aasociated with the control constraint (8-11).

The necessary conditions for optimality which correspond to a weak form of the maximum principle and which are identical to those derived from a first order perturbation analysis of P_1 (Appendix B) are then:

$$\frac{\partial \bar{H}}{\partial k} = \int_0^1 \left(p \frac{\lambda K F \cdot \psi}{kw} - \mu f g\right) dz \begin{cases} = 0 \text{ on } S_1 \\ \geq 0 \text{ when } k^+(t) = k^* \\ \leq 0 \text{ when } k^+(t) = k_w \end{cases} \tag{8-17}$$

and

$$\frac{\partial H}{\partial w} = \int_0^1 -\frac{\lambda K F \psi}{w^2}\, dz + [x_1(t) - x_0(t)] - \kappa \begin{cases} = 0 \text{ on } S_2 \\ \geq 0 \text{ when } w^+(t) = w^* \\ \leq 0 \text{ when } w^+(t) = w_* \end{cases} \quad (8\text{-}18)$$

where S_1 and S_2 correspond to these parts of the optimal control policies where $k^+(t)$ and $w^+(t)$ respectively are unconstrained.

8.2 Properties of the Optimal Control

From (8-13) and (8-5) it follows that

$$\frac{\partial \lambda F}{\partial z} = \mu k f' g F \quad \text{for all } z \in [o,1] \; ; \; t \in [o,1] \quad (8\text{-}19)$$

Assuming $F \neq 0$ for all $x \in [x_0, x_1]$, Equation (8-19) can also be written as

$$\mu k f' g = \frac{1}{F} \frac{\partial \lambda F}{\partial z} \quad (8\text{-}20)$$

Considering (8-6), (8-14) and (8-20) we also have

$$\frac{\partial \mu k f g}{\partial t} = -\frac{\lambda K F}{w} kfg + \mu f g \frac{dk}{dt} + \frac{1}{F} \frac{\partial \lambda F}{\partial z} \frac{\partial x}{\partial t} \quad (8\text{-}21)$$

By substituting

$$\frac{\lambda K F}{w} kfg = -\frac{\lambda K F}{w} \frac{\partial \psi}{\partial t} = -\frac{\lambda F}{w} \frac{\partial K \psi}{\partial t} + \frac{\lambda F \psi}{w} \frac{dK}{dt} \quad (8\text{-}22)$$

into (8-21), noting that

$$\frac{dK}{dt} = \frac{pK}{k}\frac{dk}{dt} \tag{8-23}$$

and integrating (8-21) over the z-domain gives

$$\frac{d}{dt}\int_0^1 \mu kfg\,dz = \int_0^1 \frac{\lambda F}{w}\frac{\partial K\psi}{\partial t}\,dz - \frac{dk}{dt}\int_0^1 (p\frac{\lambda K F \psi}{kw} - \mu fg)dz$$

$$+ \int_0^1 \frac{1}{F}\frac{\partial \lambda F}{\partial z}\frac{\partial x}{\partial t}\,dz \tag{8-24}$$

The last term in (8-24) can be integrated by parts to give:

$$\int_0^1 \frac{1}{F}\frac{\partial \lambda F}{\partial z}\frac{\partial x}{\partial t}\,dz = \lambda\frac{dx}{dt}\Big|_0^1 - \int_0^1 \lambda F(\frac{1}{F}\frac{\partial^2 x}{\partial z \partial t} - \frac{F'}{F^2}\frac{\partial x}{\partial t}\frac{\partial x}{\partial z})dz \tag{8-25}$$

Using (8-5), (8-15) and taking $dx_0(t)/dt = 0$, Equation (8-25) becomes:

$$\int_0^1 \frac{1}{F}\frac{\partial \lambda F}{\partial z}\frac{\partial x}{\partial t}\,dz = w\frac{dx_1}{dt} - \int_0^1 \frac{\lambda F}{w}\frac{\partial K\psi}{\partial t}\,dz + \frac{1}{w^2}\frac{dw}{dt}\int_0^1 \lambda K F \psi dz \tag{8-26}$$

Substituting (8-26) and (8-17) into (8-24) and noting that $\frac{dk}{dt}\frac{\partial H}{\partial k} = 0$ at the optimum for all t $\in[0,1]$ we get

$$\frac{d}{dt}\int_0^1 \mu kfg\,dz = w\frac{dx_1}{dt} + \frac{1}{w^2}\frac{dw}{dt}\int_0^1 \lambda K F \psi dz \tag{8-27}$$

for all t $\in[0,1]$.

Let $D = (t_1,t_2) \subset [0,1]$ be the time interval over which both

optimal control policies $k^+(t)$ and $w^+(t)$ are unconstrained simultaneously.

Property 1:

> Provided:
>
> (i) $\frac{dx_o}{dt} = 0$
>
> (ii) $P \neq 1$
>
> (iii) D is non-empty
>
> then
>
> $w(x_1 - x_o - \kappa) = \text{constant on D}$

Proof:

Substituting $\partial\bar{H}/\partial w = 0$ on S_2 from (8-18) into (8-27) gives:

$$\frac{d}{dt}\int_o^1 \mu k f g dz = w\frac{dx_1}{dt} + (x_1 - x_o - \kappa)\frac{dw}{dt} \quad \text{on } S_2 \tag{8-28}$$

From (8-18) we also can write,

$$\frac{d}{dt}\int_o^1 \frac{\lambda K F \psi}{w} dz = \frac{d}{dt}[w(x_1 - x_o - \kappa)] \quad \text{on } S_2 \tag{8-29}$$

From (8-17) we get

$$\frac{d}{dt}\left(k\frac{\partial\bar{H}}{\partial k}\right) = \frac{d}{dt}\int_o^1 \frac{p \lambda K F \psi}{w} dz - \frac{d}{dt}\int_o^1 \mu k f g dz = 0 \quad \text{on } S_1 \tag{8-30}$$

Hence from (8-28), (8-29) and (8-30), using $dx_0/dt = 0$, it follows that

$$(p - 1) \frac{d}{dt}.[w(x_1 - x_0 - \kappa)] - 0 \quad \text{on } D \tag{8-31}$$

which for $p \neq 1$ implies

$$w(x_1 - x_0 - \kappa) = \text{constant on } D \tag{8-32}$$

Q.E.D.

8.2.1 Conversion Independent Decay: $f' = 0$

For the special case where $f' = 0$, Equation (8-19) becomes

$$\frac{\partial \lambda^* F}{\partial z} = 0 \tag{8-33}$$

which from (8-15) gives us

$$\lambda F = w F_1 \tag{8-34}$$

We now can proceed to prove the following property:

Property 2:

Provided;

(i) $\frac{dx_0}{dt} = 0$

(ii) $p \neq 1$

(iii) $f' = 0$ and $F' \neq 0$

(iv) D is non-empty

then

$$\frac{dx_1}{dt} = \frac{dw}{dt} = 0 \quad \text{on } D$$

Proof:

From Property 1 and Equation (8-29) we have

$$\frac{d}{dt} \int_0^1 \lambda F \frac{K\psi}{w} dz = 0 \quad \text{on } D \tag{8-35}$$

Using (8-34) this can also be written as

$$\frac{d}{dt} \int_0^1 \lambda F \frac{K\psi}{w} dz = (w F_1' \frac{dx_1}{dt} + F_1 \frac{dw}{dt}) \int_0^1 \frac{K\psi}{w} dz$$

$$+ w F_1 \frac{d}{dt} \int_0^1 \frac{K\psi}{w} dz = 0 \quad \text{on } D \tag{8-36}$$

Since we assumed that F does not become zero for any $x \in [x_0, x_1]$, Equation (8-5) can be integrated as follows:

$$\int_{x_0}^{x_1} \frac{dx}{F} = \int_0^1 \frac{K\psi}{w} dz \tag{8-37}$$

Differentiating both sides of (8-37) using Leibnitz's rule gives us for $dx_0/dt = 0$

$$\frac{1}{F_1} \frac{dx_1}{dt} = \frac{d}{dt} \int_0^1 \frac{K\psi}{w} dz \tag{8-38}$$

Substituting (8-38) into (8-36) gives

$$\left(\int_0^1 F_1' K \psi dz \right) \frac{dx_1}{dt} + \frac{dw}{dt} F_1 \int_0^1 \frac{K\psi}{w} dz + w \frac{dx_1}{dt} = 0 \quad \text{on } D \tag{8-39}$$

However, from (8-34) and (8-18) we also have

$$F_1 \int_0^1 \frac{K\psi}{w} dz = \int_0^1 \frac{\lambda F K \psi}{w^2} dz = x_1 - x_0 - \kappa \quad \text{on } S_2 \tag{8-40}$$

Substituting (8-40) into (8-39) and using the result of Property 1, Equation (8-39) becomes

$$(F_1' K \int_0^1 \psi dz) \frac{dx_1}{dt} = 0 \quad \text{on } D \tag{8-41}$$

Hence, unless $F_1' = 0$, (8-41) implies

$$\frac{dx_1}{dt} = 0 \quad \text{on } D \tag{8-42}$$

From Property 1 we also have

$$(x_1 - x_0 - \kappa) \frac{dw}{dt} + w \frac{dx_1}{dt} = 0 \quad \text{on } D \tag{8-43}$$

which from (8-42) implies

$$(x_1 - x_0 - \kappa) \frac{dw}{dt} = 0 \quad \text{on } D \tag{8-44}$$

The term $(x_1 - x_0 - \kappa)$ cannot be zero since from (8-40) this

would imply that $F_1 = 0$ and this has been excluded.

Therefore

$$\frac{dw}{dt} = 0 \quad \text{on } D \tag{8-45}$$

Q.E.D.

Remark:

Since for Property 1 and Property 2 we assumed the set D to be non-empty, we cannot employ these results efficiently in the calculation of the optimal control policies as we do not know in advance if there will exist a non-empty set D for the given problem. The main value of these properties however, lies in the fact that for the problems where they are applicable, they provide us with an additional check on the calculated optimal control policies in case both $k^+(t)$ and $w^+(t)$ are unconstrained simultaneously over a finite time interval.

8.3 Numerical Procedure

For the given boundary control problem (8-5) - (8-11), the state and adjoint equations can again be integrated as ordinary differential equations along lines which are parallel with the coordinate axes.

The optimal inlet temperature control $k^+(t)$ is calculated iteratively by hill-climbing on the boundary hamiltonian $\bar{H}$. The procedure to update the control k(t) at each iteration is identical to the one used in Chapter 6 for inlet temperature control only.

Since we have to calculate two boundary control policies, the control variable w(t) can also be adjusted at each iteration step. By also using the gradient method, the control w(t) can be updated to w(t) + δ w(t) where δ w(t) is given by

$$\delta w(t) = \eta\left(\int_0^1 - \frac{\lambda K F \psi}{w^2}\, dz + [x_1 - x_0] - \kappa\right) \tag{8-46}$$

with η a small positive parameter.

The new control policy still has to satisfy the control constraints (8-10) and (8-11), hence δ w(t) has to be such that

$$w_* \leq w(t) + \delta w(t) \leq w^* \tag{8-47}$$

and

$$\int_0^1 \delta w(t)dt = 0 \tag{8-48}$$

Since the Lagrange multiplier κ is not known, we have to use an approximate value κ_1. The Equations (8-46) - (8-48) are similar in form to the Equations (7-52), (7-53) and (7-55) which we encountered in Chapter 7 for updating the control a(z). In order to calculate a control adjustment δ w(t) which satisfies (8-46) - (8-48) we can use a procedure which is similar to the one described in Chapter 7 for updating the control a(z).

8.3.1 Numerical Results and Discussion

Calculations have been done for two types of problems with conversion dependent catalyst decay rates.

Example 1:

The boundary control problem (8-5) - (8-11) has the following functions and parameter set:

$$F = 1 - x$$

$$f = 1 - x$$

$$g = \psi^{0.5}$$

$$p = 0.5 \qquad (8\text{-}49)$$

$$x_0(t) = 0 \; ; \; \psi_0(z) = 1$$

$$k^* = k[T^*] = k[900] \; ; \; k_* = k[T_*] = k[700]$$

The pre-exponential constants for the rate constants K and k are identical to the ones used in the two previous chapters. The value of L in Equation (8-2) was taken as unity. Optimal control policies have been calculated for the problem with this set of parameters and different values of the total operating time t_f. The different values of t_f, given as fractions of a 25 day operation, are t_f = .72, .60, .57, .54, .52 and .50.

In order to compare the optimal values of the objective function for different values of t_f, we made certain that in all cases an equal amount of reactants was processed. This was accomplished by choosing

the value of v_{av} as

$$v_{av} = 1/t_f \tag{8-50}$$

(for instance, $v_{av} = 2.$ for $t_f = .5$).

We also can define identical upper and lower constraints on the flow rate for the problems with different t_f by writing (8-10) and (8-11) as follows:

$$0 \leq w(t) \leq 2t_f \tag{8-51}$$

and

$$\int_0^1 w(t)dt = 1 \tag{8-52}$$

The best calculated boundary control policies are plotted as $T^+(t)$ and $v^+(t)(v^+(t) = v_{av}\, w^+(t))$ in Figure 8-1 for different values of t_f.

A typical exit conversion profile $x_1^+(t)$ corresponding to the best calculated boundary control policies is illustrated in Figure 8-2 for the case with $t_f = .57$.

Although the difference in the values of the objective function P_1^+, evaluated at the optimum, and P_{1U}, corresponding the best constant boundary control policies, can be significant for a given value of t_f (for instance $P_1^+ = .955327$ and $P_{1U} = .9206496$ with $t_f = .57$), it is more realistic to compare the performances of the reactor for different values of t_f on the basis of production per time unit. We therefore, define the objective function P_2 as

$$P_2 = P_1^+ v_{av}/(t_f + t_D) \qquad (8\text{-}53)$$

where P_1^+ is the value of P_1, defined in (8-8), evaluated at the optimal policies $k^+(t)$ and $w^+(t)$ and where t_D accounts for the down-time of the reactor. The calculated values of P_2 for the different values of t_f and with $t_D = 0, .5, .6$ and $.7$ are tabulated in Table 8-1.

From the numerical results obtained for Example 1, the following observations can now be made:

1) For sufficiently large values of t_f, the optimal control policies $k^+(t)$ and $w^+(t)$ can indeed be simultaneously unconstrained over a finite time interval D (Figure 8-1).
2) On D, the calculated optimal policies do comply with the result of Property 1.
3) Although Property 2 only has been proven for $f' = 0$, the results of this Property have shown to be valid also for this problem.
4) If no reactor down-time is taken into consideration, the maximum production per time unit is obtained for the case where $w^+(t)$ is totally upper constrained (i.e., the flow rate of the fluid stream is kept as high as possible).
5) From Table 8-1, we see that in order to obtain a maximum of P_2 for which $w^+(t)$ is not totally constrained, we need to consider a down-time t_D which is larger than the total operating time t_f. Hence, for all realistic situations, the optimum of this problem will occur at $w^+(t) = w^*$ for all $t \in [0,1]$.

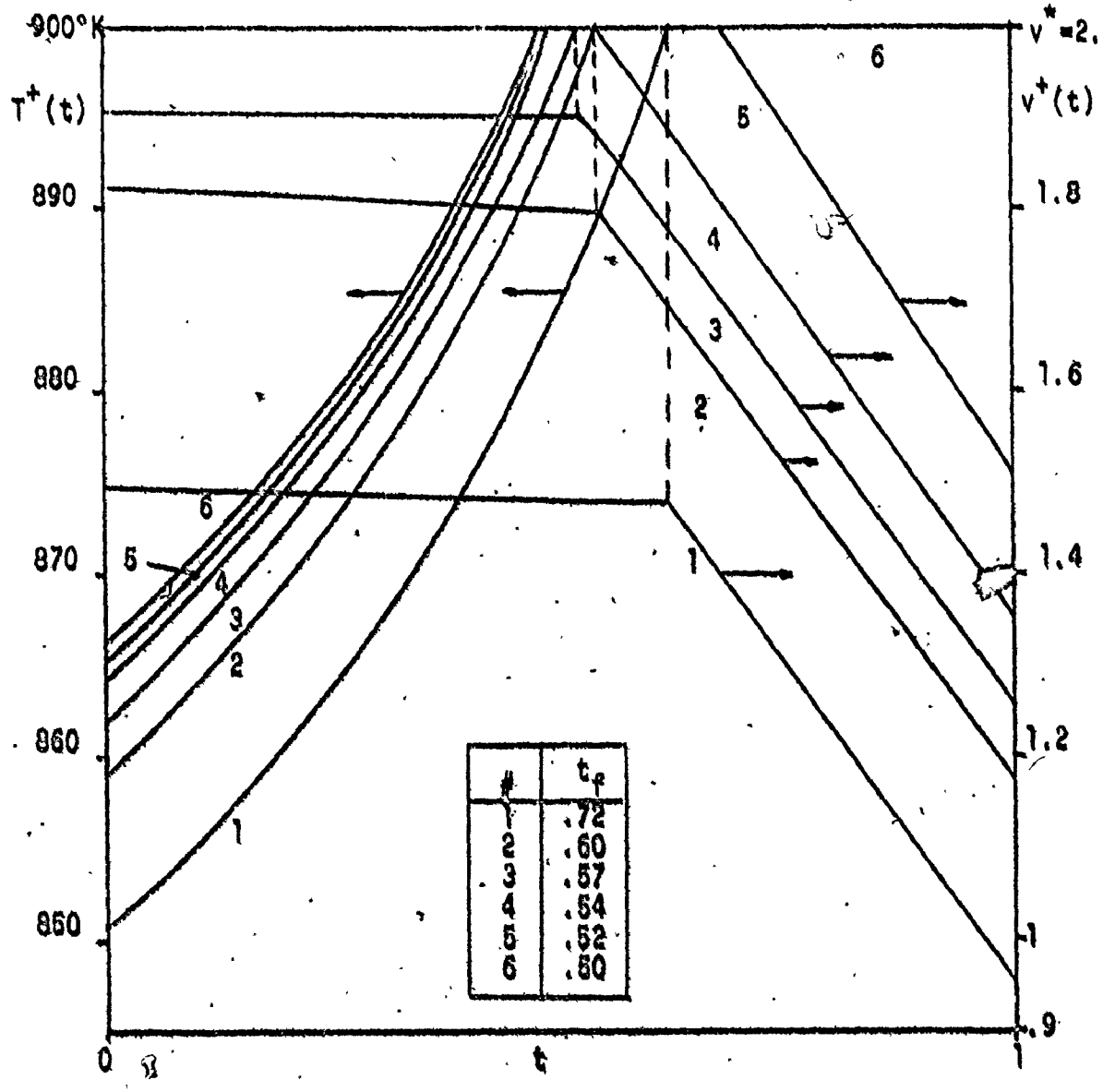

Figure 8-1: Optimal control policies $T^*(t)$ and $v^*(t)$ in Example 1 for different values of t_f.

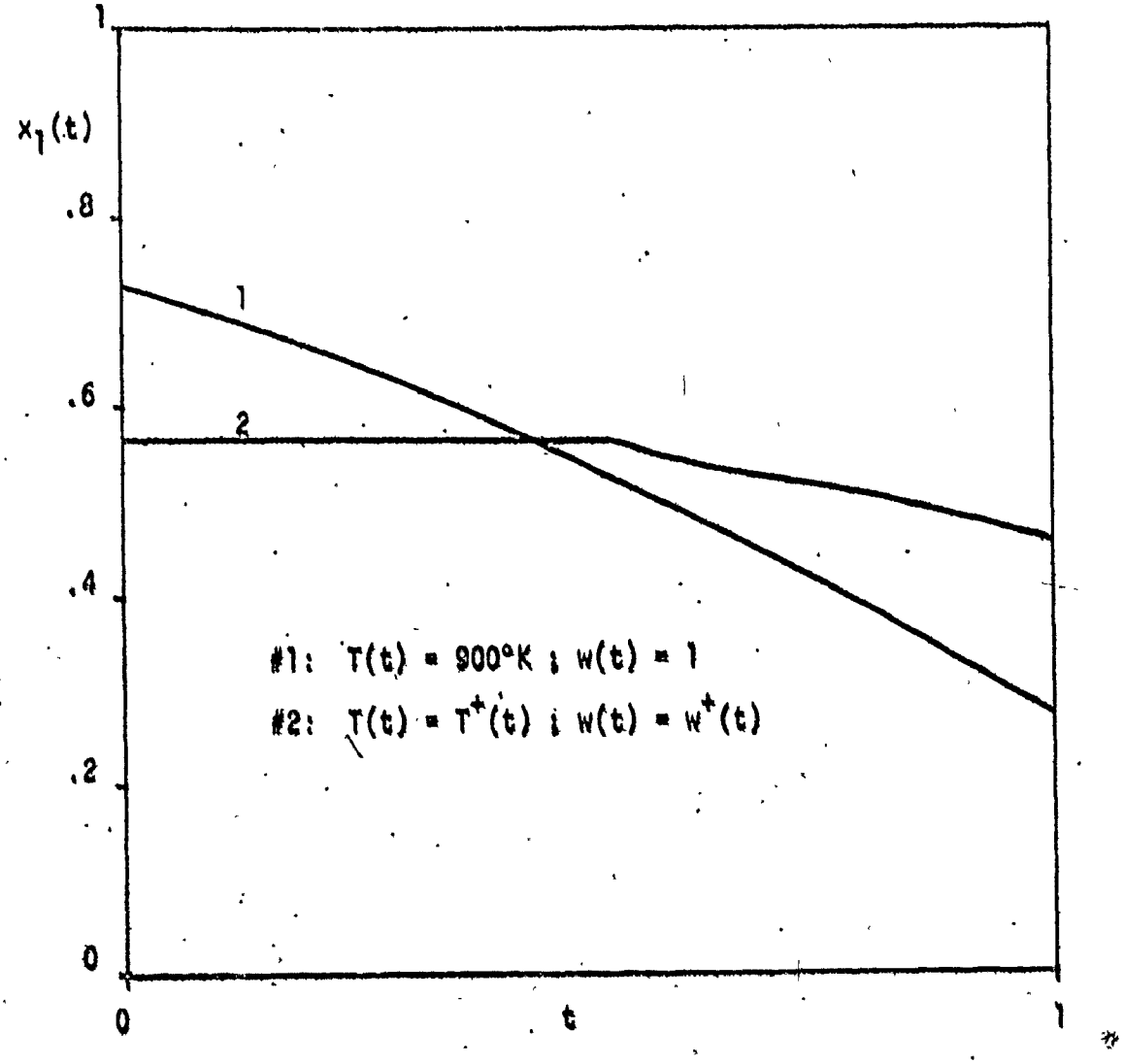

Figure 8-2: Example of the exit conversion policy $x_1(t)$ for optimal and uniform control policies in Example 1 with $t_f = .57$.

Table 8-1: Values of the objective function P_2 for different values of t_f and t_D in Example 1.

t_f	$P_2(t_D = 0)$	$P_2(t_D = .5)$	$P_2(t_D = .6)$	$P_2(t_D = .7)$
.72	.834457	.492466	.455158	.423105
.60	.927970	.506165	.463985	.428294
.57	.955327	.508913	.465416	.428769
.54	.984698	.511234	.466389	.428777
.52	1.004770	.512236	.466500	.428263
.50	1.024703	.512362	.465774	.426960

Example 2:

The functions F, f and g in this example are

$$F = (1 - x)^2$$

$$f = (1 - x)^{.5}/x \qquad (8\text{-}54)$$

$$g = \psi^2$$

The set of parameters is chosen identical to this of Example 1 except for the constraint (8-51) which is now taken as

$$0 \leq w(t) \leq t_f \qquad (8\text{-}55)$$

The optimal policies $k^+(t)$ and $w^+(t)$ have been calculated for values of t_f equal to 1.32, 1.29, 1.26, 1.20, 1.16, 1.08, 1.04 and 1.

A selection of some of the best calculated policies, plotted as $T^+(t)$ and $v^+(t)$ ($v^+(t) = v_{av}\, w^+(t)$,) is given in Figure 8-3. A typical optimal exit conversion policy $x_1^+(t)$ is shown in Figure 8-4 for the case with $t_f = 1.20$. The values of P_2, defined by (8-53), are tabulated in Table 8-2 for the different values of t_f and with $t_D = 0$, 3.9, 4.0 and 5.0.

From Figure 8-3 we observe that even for relatively large values of t_f, we did not encounter an interval D over which both optimal controls are simultaneously unconstrained.

This example is also exceptional in the sense that as t_f becomes larger, the region S_1 over which $k^+(t)$ is unconstrained diminishes. Note however, that since the time scale in Figure 8-3 is normalized, the graphs of $k^+(t)$ in Figure 8-3 show an enlarged view of this effect. On

the real time axis however, this effect is still substantial. For instance for $t_f = .1$ (25 days), we found a value of S_1 corresponding to 14 days, whereas for $t_f = 1.29$ (32.25 days) we obtained a time interval of 11.6 days for S_1.

From Table 8-2, we notice that in order to have an optimal policy $w^*(t)$ which is not totally constrained, the down-time t_D has to be extremely large. Therefore, as was the case in Example 1, the optimal flow rate of the fluid stream will have to be as large as possible for all practical situations.

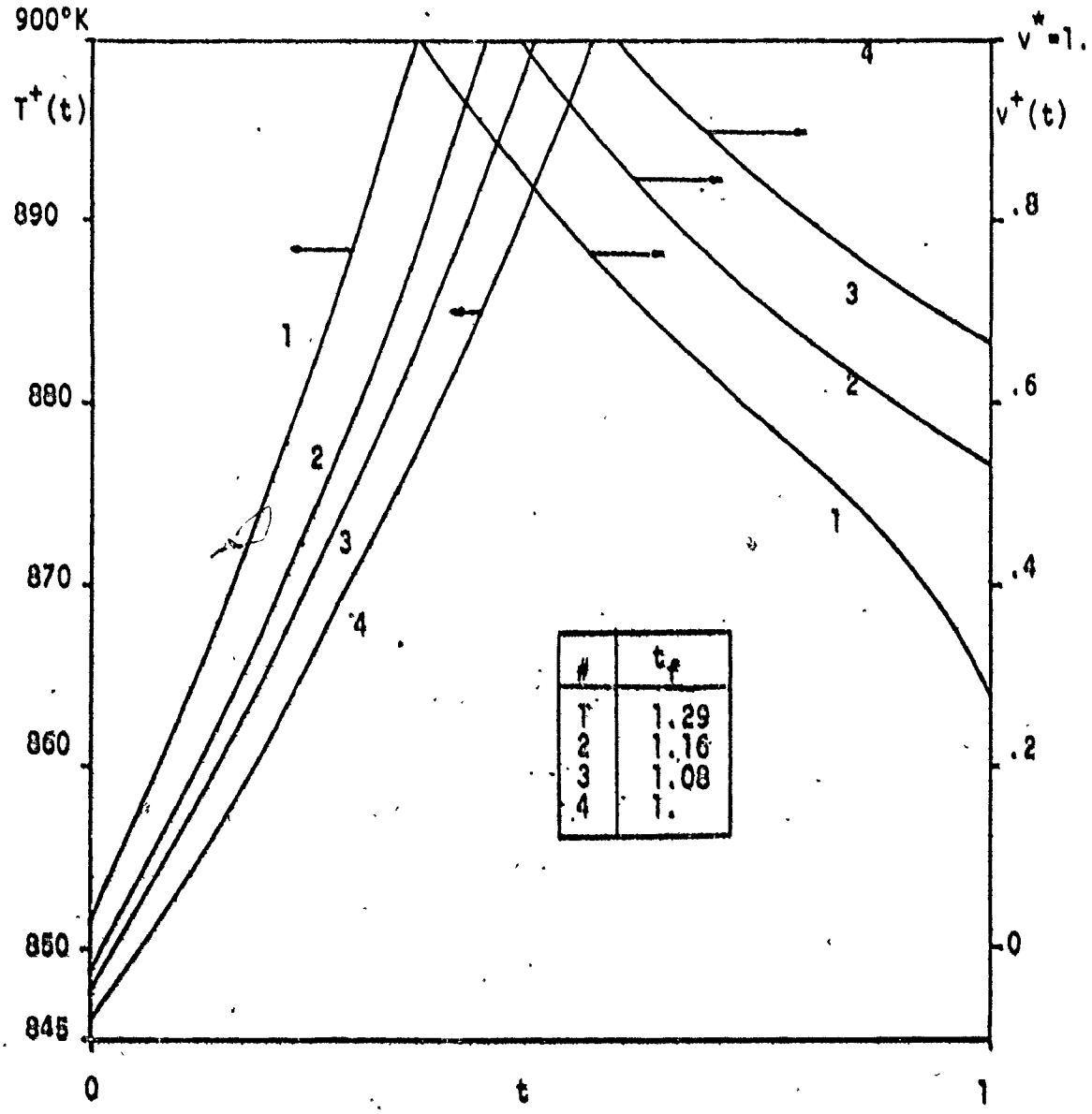

Figure 8-3: Optimal control policies $T^+(t)$ and $v^+(t)$ in Example 2 for different values of t_f.

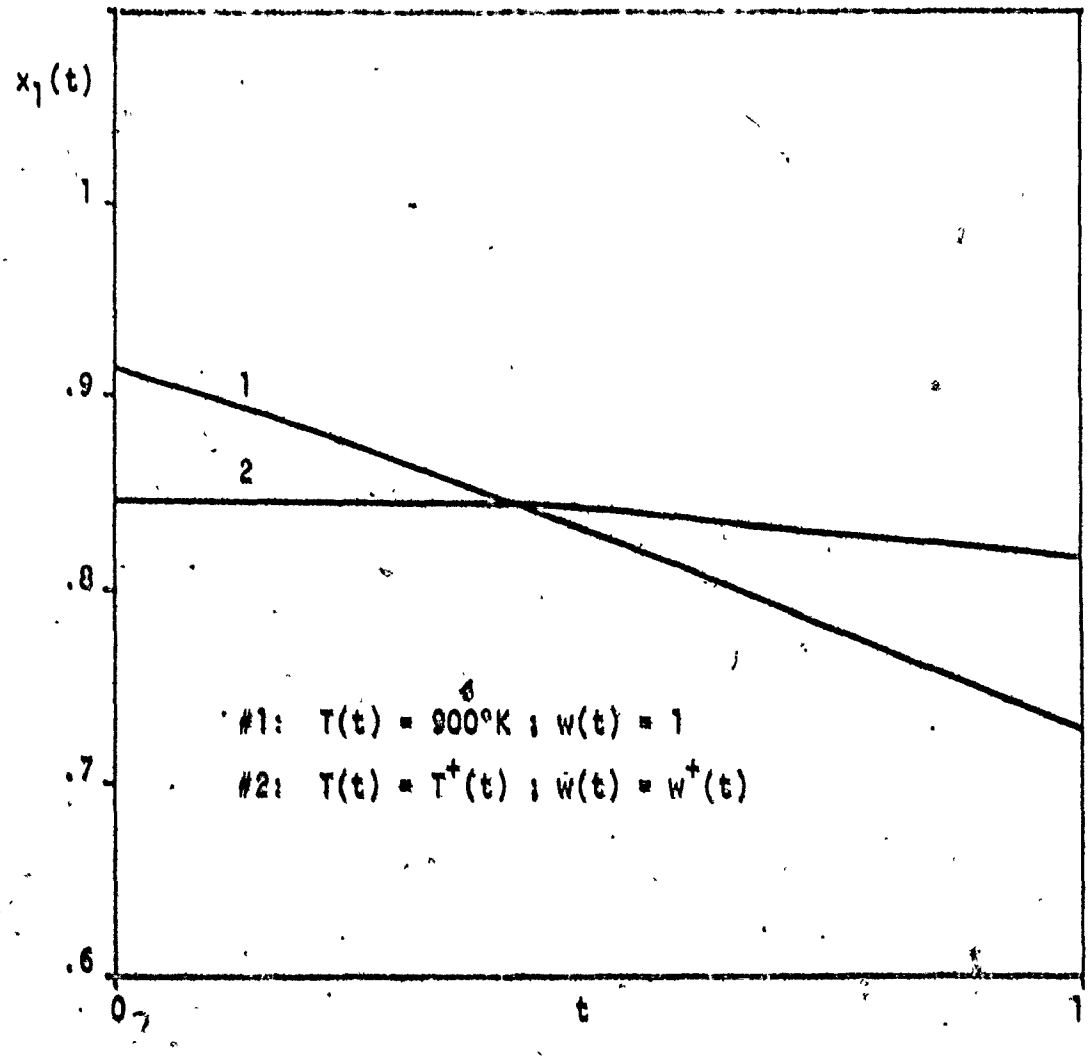

Figure 8-4: Example of the exit conversion policy $x_1(t)$ for optimal and uniform control policies in Example 2 with $t_f = 1.20$.

Table 8-2: Values of the objective function P_2 for different values of t_f and t_D in Example 2.

t_f	$P_2(t_D = 0)$	$P_2(t_D = 3.9)$	$P_2(t_D = 4)$	$P_2(t_D = 5)$
1.32	.566027	.143133	.140443	.118221
1.29	.577797	.143614	.140899	.118499
1.26	.590162	.144109	.141370	.118787
1.20	.616371	.145028	.142239	.119298
1.16	.634455	.145448	.142629	.119475
1.08	.674147	.146201	.143323	.119750
1.04	.695443	.146409	.143504	.119745
1.	.717431	.146414	.143486	.119572

CHAPTER 9

SUMMARY AND CONCLUSIONS

A maximum principle formulation has been used in the study of optimal boundary control of chemical fixed-bed tubular reactors with slowly decaying catalyst. One of the most important findings in this study is that we have been able to prove that a strong form of the maximum principle for boundary control of hyperbolic distributed parameter systems cannot be applied for boundary control problems where the direction of the lines along which the control variable remains unchanged coincides with one of the characteristic directions of the system.

It is shown in Chapter 4 that for a particularly chosen boundary control problem, denoted Problem Π_b, the optimal piecewise-continuous control policy, whose existence and uniqueness has been proven, does not satisfy the necessary conditions formulated by a maximum principle formulation which requires the boundary hamiltonian function to reach an absolute maximum with respect to the boundary control at the optimum.

For the Problem Π_e, which is similar to Problem Π_b but where the control characteristic does not coincide with any of the state characteristics, it is indicated by numerical results that there does not seem to exist an optimal boundary control policy which belongs to

the class of piecewise continuous functions. The numerical results indeed suggest that the optimal boundary control policy for this particular problem is a relaxed control which chatters infinitely fast between two piecewise continuous controls.

For the quasi-steady state catalytic reaction-deactivation system where a single irreversible reaction occurs, the problems of choosing the optimal inlet temperature policy, the initial relative catalyst activity profile and the inlet fluid flow rate into the reactor have been studied. The integrated average initial catalyst activity and the total amount of fluid to be processed were fixed and the control variables were constrained by upper and lower limits. The rate of reaction and the rate of catalyst deactivation were both considered to be expressible as a product of separate functions of temperature, relative catalyst activity and conversion. The temperature inside the reactor was taken either as adiabatic or as being uniform along the axis of the reactor.

A weak form of the maximum principle, which requires the boundary hamiltonian to be stationary when the optimal control is unconstrained and to reach a local maximum with respect to the control when the optimal control is on one of its constraints, has been used in formulating necessary conditions for optimality of the boundary control policies. From these necessary conditions, certain properties of the optimal control policies have been derived.

In Chapter 6 we have proven that the "constant exit conversion

property", which had been proven earlier for conversion independent decay, remains valid for the optimal inlet temperature policy of problems with conversion-dependent decay rate expressions and for which the decay rate is of first order (i.e., m = 1). The numerical results however, show the constant exit conversion property still to hold for all problems which have been investigated and for which the decay rate was not first-order. An analytical proof of this property for general orders of decay has not been found.

In the study of the optimal initial catalyst activity distribution, it is proven in Chapter 7 that for first order decay rate expressions (i.e., m = 1), the performance of the reactor is not affected by the initial relative catalyst activity distribution provided the integrated average activity is specified.

For conversion independent decay, it is shown that for $m > 1$ ($m < 1$), an initial catalyst load with uniform activity is better (worse) than a mixture of two batches of catalyst, both of the same type but with different initial activities; independently of how any such mixture is put into the reactor at time zero.

Numerical calculations for problems with conversion-dependent decay and decay rate expressions which are not of first order show that the optimal composition of the initial catalyst load, which consists of equal amounts of two batches of catalyst with different activities, is of a bang-bang nature. We also found that the sign of the product $(m - 1)f'$ determines which catalyst is loaded first into the reactor. For instance, in the cases which have been studied, it was found that

whenever $(m - 1)f'$ was positive (negative), the catalyst with the highest (lowest) relative activity should be placed in the first half of the reactor.

In Chapter 8 we have considered the problem of simultaneously choosing the optimal inlet temperature policy and the optimal inlet fluid-flow rate for problems with fixed total operating time and a fixed amount of fluid to be processed. For conversion independent decay, it has been proven that whenever both optimal controls are simultaneously unconstrained over a finite time interval, the fluid flow rate and the exit conversion then remain constant over that time interval provided the inlet conversion $x_0(t)$ remains constant and the reaction does not go to completion.

It is shown numerically that for a particular problem with conversion dependent decay, this property still remains valid.

If, however, the performance of the reactor is measured as production per time unit, we found that for those problems which have been investigated, the best performance was obtained by choosing the total operating time such that the inlet flow rate was always kept at its upper constraint. The totally constrained flow rate policy ceased to be optimal only when unreasonably large values of the reactor downtime were used in the calculation of the reactor performance.

9.1 Recommendations for Future Work

Although this reaction-deactivation process lends itself easily to the formulation of a large variety of optimal control studies, we

feel that in view of the present study, a further systematic investigation is required to either prove or contradict the following two conjectures:

Conjecture 1: The strong form of the maximum principle for boundary control of hyperbolic distributed parameter systems is also invalid for problems where the control characteristics do not coincide with any of the state characteristics of the system.

Conjecture 2: For the given reaction-deactivation process, the optimal constant exit conversion property remains valid for conversion dependent decay rate expressions where the order of decay is not equal to 1.

LIST OF SYMBOLS

a_i	real constant coefficient in system (3-1)
$a(z)$	boundary control variable for catalyst distribution in Chapter 7
A	constant defined by (5-29)
$A(t)$	function defined by (7-14)
b_i	real constant coefficient in system (3-1)
c	positive constant in (7-7)
c_i	molar concentration of species i in a chemical reaction
c_p	mean heat capacity
C	positive constant in (6-49)
C^*	constrained control policy characterized by condition (6-15)
C_*	constrained control policy characterized by condition (6-16)
d	constant in (7-22)
D	function defined by (7-51)
D_i	value of D at i^{th} grid point along the z-axis
D	region where both $k^+(t)$ and $w^+(t)$ are unconstrained (Chapter 8)
E	closed domain along the z-axis $[z_0, z_f]$
E_R	reaction activation energy
E_c	catalyst deactivation energy
$f_i(z,t,x,u)$	function in system (3-1)
$f(\phi,k)$	velocity function (4-19)
$\bar{f}(\phi,\bar{k})$	velocity function corresponding to the relaxed control policy $\bar{k}(t)$

$f(\alpha\phi, k^*)$	pseudo-relaxed velocity function (4-45)
$f, f[x]$	conversion dependent function in decay rate expression
$F, F[x]$	conversion dependent function on reaction rate expression
F', f'	first derivatives of F and f with respect to x
$\bar{F}[x], \bar{f}[x]$	conversion dependent functions for an adiabatic reactor (A-13) and (A-15)
$F_1, F_1(x_0, x_1)$	function defined in (6-24)
$F(K\phi), F(x_0, K\phi)$	function defined in (6-29)
F'	first derivative of $F(K\phi)$ with respect to $K\phi$
$g, g[\psi]$	activity dependent function in decay rate expression
g'	first derivative of g with respect to ψ
$g(\phi, k)$	velocity function (4-20)
$\bar{g}(\phi, \bar{k})$	velocity function corresponding to the relaxed control policy $\bar{k}(t)$
$g(\alpha\phi, k^*)$	pseudo-relaxed velocity function (4-46)
G, G_1, G_2	integrands in the objective function J (3-4)
$g_1(K\phi)$	function defined in (6-31)
$g(K\phi), g(x_0, K\phi)$	function defined in (6-34)
g'	first derivative of $g(K\phi)$ with respect to $K\phi$
$H, H(z, t, x, \lambda, \mu)$	scalar hamiltonian function (3-6)
H_1, H_2	boundary hamiltonians (3-15), (3-17)
$\bar{H}$	boundary hamiltonian
H_ℓ	lumped hamiltonian function (4-25)
$H_{\ell c}$	value of H_ℓ corresponding to t_{fc}
$M(K\phi)$	function defined in (6-49)

I	closed time domain $[t_0,t_f]$
J	objective function (3-4)
J	defined in (A-3)
J'	defined in (A-9)
$k,k[T]$	catalyst deactivation rate constant also taken as control variable (5-21)
$k,k(t)$	boundary control policy
$\bar{k},\bar{k}(t)$	relaxed control policy
$k_i(t)$	i^{th} control policy in algorithm (4-37)
k_0	pre-exponential factor in (5-15)
$k^\dagger(t)$	deactivation rate constant of Arrhenius form (5-15)
$K,K[T]$	reaction rate constant in dimensionless form (5-20)
K_0	pre-exponential factor in (5-5)
$K^\dagger[T]$	reaction rate constant of Arrhenius form (5-5)
$\overline{K\phi},\underline{K\phi}$	maximum and minimum values of $K\phi$ defined by (6-55) and (6-56)
L	length of catalyst bed
L	set of endpoints defined in Figure 4-2
L	function defined by (7-24)
m	order of deactivation
n	order of a single irreversible reaction
N	number of discrete time intervals along the z-axis, Section 7.4.2
N	half the number of switches in a bang-bang policy, Section 4.4.3

p	ratio of E_R/E_c
P	performance index (5-31)
P_1	performance index (8-8)
P_2	performance index (8-51)
q	defined as $q = 1 - m$ in (7-13)
r	exponent of $(1 - x)$ in decay rate expression
R	universal gas constant
R_i	molar rate of formation of species i in a chemical reaction
s_1, s_2	characteristic directions associated with the state variables x and ψ
S	unconstrained control policy associated with condition (6-14)
S_1, S_2	unconstrained control policies associated with conditions (8-17) and (8-18)
t	independent time variable in system (3-1)
t	dimensionless time $t \in [0,1]$
t'	real time since start-up $t' \in [0, t_f]$
t_o	specified initial or starting time
t_f	specified final time
t_{fc}	critical final time
t_θ	mean space time $t_\theta = L/v$
$T, T(t)$	temperature in degrees Kelvin
T_{max}, T_{min}	maximum and minimum allowable temperature in an adiabatic reactor

u	control vector in system (3-1)
$u_k(z,t)$	distributed control variable
$u_k(z)$	uniform or boundary control variable
$u_k(t)$	uniform or boundary control variable
U	admissible control region
$v, v(t)$	molar fluid flow rate
v_{av}	time average linear fluid flow rate
$\hat{V}(\phi)$	extended velocity set (4-21)
$V_R(\phi)$	pseudo-relaxed velocity set (4-47)
$w(t)$	dimensionless fluid flow rate and boundary control variable (8-4)
$W(k)$	control set (4-44)
$x, x(z,t)$	state variable, conversion of a single irreversible chemical reaction
$x_0(z)$	conversion along the axis of the reactor at initial time
$x_0(t)$	inlet conversion into the reactor
$x(1,t), x_1(t)$	exit conversion out of the reactor
x_f	state variable in system (3-1)
Y	function defined by (7-27)
z	independent variable in system (3-1)
z	dimensionless axial distance in the reactor $z \in [0,1]$
z'	real distance along the axis of the reactor $z' \in [0,L]$
z_0	starting point of the z-domain, inlet to the reactor bed
z_f	endpoint of the z-domain, end of the catalyst bed

α	constant in (6-48)
$a(z)$	initial condition for x in system (3-1)
$\alpha(t)$	element of the relaxed control policy $\bar{k}(t)$ (4-23), (4-24)
$\beta(t)$	boundary condition for x in system (3-1)
$\gamma,\gamma(t)$	lumped adjoint variable (4-26)
δt	finite interval in time
δk	small admissible control variation in k(t)
δw	small admissible control variation in w(t)
$\delta w(t)$	admissible control variation in w(t)
$\delta a(z)$	admissible control variation in a(z)
δP_1	variation in the objective function (B-6)
δx	variation in the conversion x
$\delta x_1(t)$	variation in the exit conversion $x_1(t)$
$\delta\psi$	variation in the catalyst activity ψ
ΔH_R	heat of reaction
Δt	finite interval in time
Δz	finite interval in distance
e,e_1,e_2	non-negative constant parameters
λ_j	adjoint variable in system (3-6)
$\lambda,\lambda(z,t)$	adjoint variable to the conversion x
$\mu,\mu(z,t)$	adjoint variable to the catalyst activity ψ
ν_1,ν_2	dimensionless velocities (A-1),(A-2)
κ	constant Lagrange multiplier (7-47), (8-16)
κ_1	estimated value of κ

η	small positive parameter
$\phi, \phi(t)$	average integrated catalyst activity into the reactor (4-15)
ϕ'	average integrated activity between $z = 0$ and $z' \in [0,1]$
ϕ_0	value of ϕ at initial time
$\psi, \psi(z,t)$	state variable, relative catalyst activity
$\psi_0(z)$	initial relative catalyst activity distribution
$\psi_1(z,t)$	relative catalyst activity for catalyst 1
$\psi_{10}(z)$	initial relative catalyst activity for catalyst 1
ψ_{u0}	initial uniform catalyst activity
Ω	rate of reaction (5-2)

Superscripts

+	refers to values corresponding to optimal policies
*	refers to values corresponding to control policies which are at their upper constraint

Subscripts

z	refers to partial derivation with respect to z
t	refers to partial derivation with respect to t
*	refers to values corresponding to control policies which are at their lower constraint

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APPENDIX A

ADIABATIC vs. UNIFORM TEMPERATURE REACTOR

The mass balance Equation (5-22) for a tubular fixed-bed reactor where a single irreversible reaction A → B takes place is given by

$$x_t + \nu_1 x_z = \Omega(T,x,\psi) = K[T]\ F[x]\psi \tag{A-1}$$

where x is the conversion, Ω the rate of reaction and ν_1, the dimensionless velocity factor. We consider ν_1 to remain constant.

The corresponding energy equation in molar units can then be written as

$$T_t + \nu_2\ T_z = J\ \Omega \tag{A-2}$$

where ν_2 is the velocity factor for the temperature T(z,t) and

$$J = -\frac{\Delta H_R}{c_p} \tag{A-3}$$

where ΔH_R is the heat of reaction and c_p is the mean heat capacity. We also consider ν_2 to be constant.

In general the velocity factor ν_1 will be larger than ν_2.

Unless a large variation of the inlet conversion $x_0(t)$ or the inlet temperature $T_0(t)$ occurs over a small time interval, the quasi-steady state approximation is often valid for reactor systems with

slowly decaying catalyst. The Equations (A-1) and(A-2) under quasi-steady state assumptions then become:

$$\nu_1 x_z = \Omega \tag{A-4}$$

$$\nu_2 T_z = J \Omega \tag{A-5}$$

Eliminating Ω between these two expressions then gives

$$\frac{dT}{dx} = J \frac{\nu_1}{\nu_2} \tag{A-6}$$

As the heat of reaction ΔH_R and the heat capaicty c_p are both functions of T, their ratio is often nearly constant over the temperature range inside the reactor. In case J can be considered constant (A-6) leads to

$$T - T_o = J \frac{\nu_1}{\nu_2} (x - x_o) \tag{A-7}$$

In case J/T is sufficiently constant over the operating conditions, a more practical form can be derived from (A-6) as

$$\frac{1}{T} - \frac{1}{T_o} = J' (x - x_o) \tag{A-8}$$

where $J' = - J \nu_1/(T_o T \nu_2)$. (A-9)

The temperature dependent factor in the rate expression Ω becomes then in Arrhenius form:

$$K[T] = K_o \exp(-E_R/RT) = K_o \exp(-E_R/RT_o) \exp(-E_R J'(x-x_o)/R) \qquad (A\text{-}10)$$

where K_o is the pre-exponential constant and E_R is the reaction activation energy.

Since ΔH_R is negative for exothermic reactions, J is positive (and hence J' is negative) for exothermic reactions.

Substituting (A-10) into the rate expression Ω as given in (A-1) gives

$$\Omega(T,x,\psi) = K[T_o] \exp(-E_R J'(x-x_o)/R) F[x]\psi \qquad (A\text{-}11)$$

and this can be written as

$$\Omega(T,x,\psi) = K[T_o] \bar{F}[x]\psi \qquad (A\text{-}12)$$

with

$$\bar{F}[x] = F[x] \exp(-E_R J'(x-x_o)/R) \qquad (A\text{-}13)$$

This rate expression (A-12) then gives the rate of reaction as a product of functions of the inlet temperature, the conversion and the relative catalyst activity, each of one variable only. For a uniform temperature reactor, $\bar{F}[x]$ is replaced by F[x].

In a similar way, the rate expression for the catalyst activity decay (5-24) can be written for an adiabatic reactor as follows:

$$\psi_t = - k[T_o] \bar{F}[x] g[\psi] \qquad (A\text{-}14)$$

where

$$\bar{f}[x] = f[x] \exp(- E_c J' (x-x_o)/R) \qquad (A-15)$$

This rate expression (A-14) is again similar to the one for a uniform temperature reactor where $\bar{f}[x]$ is replaced by $f[x]$.

APPENDIX B

FIRST ORDER PERTURBATION ANALYSIS

We recall the state equations (8-5) and (8-6) with initial and boundary condtions (8-7):

$$\frac{\partial x}{\partial z} = \frac{K F \psi}{w} \tag{B-1}$$

$$\frac{\partial \psi}{\partial t} = - kfg \tag{B-2}$$

$$x(o,t) = x_o(t) \; ; \; \psi(z,o) = \psi_o(z) \tag{B-3}$$

and the objective function given by (8-8):

$$P_1 = \int_0^1 [x_1(t) - x_o(t)] \, w(t)dt \tag{B-4}$$

By letting $w(t) = 1$ for all $t \in [o,1]$ in (B-1) and (B-4), we obtain the Equations (6-1) - (6-4) and (6-7) for the problem with inlet temperature control only.

In case, however, $w(t)$ is a control variable, the constraint (8-11):

$$\int_0^1 w(t)dt = 1 \tag{B-5}$$

also has to be satisfied.

We now consider small variations $\delta k(t)$ and $\delta w(t)$ of the control function $k(t)$ and $w(t)$ respectively. The corresponding variation in the objective function P_1 then can be expressed as:

$$\delta P_1 = \int_0^1 \delta([x_1(t) - x_0(t)]\, w(t))dt$$

$$+ \int_0^1 \int_0^1 \lambda[\delta(\frac{K F \psi}{w}) - \frac{\partial(\delta x)}{\partial z}]dzdt$$

$$+ \int_0^1 \int_0^1 \mu[\delta(- kfg) - \frac{\partial(\delta \psi)}{\partial t}]dzdt$$

$$- \kappa \int_0^1 \delta\, w(t)dt \qquad \text{(B-6)}$$

where λ and μ are adjoint variables and κ is a constant Lagrange multiplier.

We assume the variations δk and δw to be small enough such that in the following Taylor expansions, the second order terms can be neglected. We then can write:

$$\delta([x_1(t) - x_0(t)]\, w(t)) = [\delta x_1(t) - \delta\, x_0(t)]\, w(t)$$

$$+ [x_1(t) - x_0(t)]\, \delta\, w(t) \qquad \text{(B-7)}$$

$$\delta\left(\frac{K F \psi}{w}\right) = P \frac{K F \psi}{kw} \delta k + \frac{K F' \psi}{w} \delta x + \frac{K F}{w} \delta\psi - \frac{K F \psi}{w^2} \delta w \qquad \text{(B-8)}$$

and

$$\delta(-kfg) = -fg\delta k - kf'g\delta x - kfg'\delta\psi \qquad \text{(B-9)}$$

where F', f' and g' are the first order derivatives of F, f and g with respect to their dependent variables.

Since a variation in the controls does not affect the initial and boundary conditions (B-3) we have

$$\delta x_0(t) = 0 \; ; \; \delta \psi_0(z) = 0 \qquad \text{(B-10)}$$

We then also can derive the following expressions:

$$-\int_0^1 \lambda \frac{\partial(\delta x)}{\partial z} dz = -\lambda(1,t)\, \delta x_1(t) + \int_0^1 \delta x \frac{\partial \lambda}{\partial z} dz \qquad \text{(B-11)}$$

and

$$-\int_0^1 \mu \frac{\partial(\delta\psi)}{\partial t} dt = -\mu(z,1)\, \delta\psi(z,1) + \int_0^1 \delta\psi \frac{\partial \mu}{\partial t} dt \qquad \text{(B-12)}$$

Substituting (B-7) - (B-12) into (B-6) and rearranging gives:

$$\delta P_1 = \int_0^1 [w(t) - \lambda(1,t)]\, \delta x_1(t) dt$$

$$- \int_0^1 \mu(z,1)\, \delta\psi(z,1) dz$$

$$+ \int_0^1 \int_0^1 \delta\, x\left[\frac{\partial \lambda}{\partial z} + \frac{\lambda\, K\, F\, \psi'}{w} - \mu k f' g \right] dz\, dt$$

$$+ \int_0^1 \int_0^1 \delta\, \psi\left[\frac{\partial \mu}{\partial t} + \frac{\lambda\, K\, F}{w} - \mu k f g' \right] dz\, dt$$

$$+ \int_0^1 \left\{ \int_0^1 \left[p\, \frac{\lambda\, K\, F\, \psi}{k w} - \mu f g \right] dz \right\} \delta k\, dt$$

$$+ \int_0^1 \left\{ \int_0^1 - \frac{\lambda\, K\, F\, \psi}{w^2}\, dz + \left[x_1(t) - x_0(t) \right] - \kappa \right\} \delta w\, dt \qquad \text{(B-13)}$$

We now define

$$\frac{\partial \lambda}{\partial z} = - \frac{\lambda\, K\, F' \psi}{w} + \mu k f' g \qquad \text{(B-14)}$$

$$\frac{\partial \mu}{\partial t} = - \frac{\lambda\, K\, F}{w} + \mu k f g' \qquad \text{(B-15)}$$

$$\lambda(1,t) = w(t) \qquad \text{(B-16)}$$

$$\mu(z,1) = 0 \qquad \text{(B-17)}$$

$$H = \frac{\lambda\, K\, F\, \psi}{w} - \mu k f g \qquad \text{(B-18)}$$

We see that (B-14) - (B-18) correspond to the adjoint equations, their terminal and boundary conditions and the definition of the hamiltonian as given by the Equations (8-12) - (8-15). Similarly, for inlet temperature control only and letting $w(t) = 1$, we recover the Equations (6-8) - (6-12).

From (B-14) - (B-18), Equation (B-13) can now be written as

$$\delta P_1 = \int_0^1 [\frac{\partial}{\partial k} \int_0^1 Hdz]\delta k dt$$

$$+ \int_0^1 \{\frac{\partial}{\partial w} \int_0^1 Hdz + [x_1(t) - x_0(t)] - \kappa\}\delta w dt \qquad \text{(B-19)}$$

Since in order for P_1 to reach a maximum at the optimum where $k(t) = k^+(t)$ and $w(t) = w^+(t)$, a necessary condition for optimality is:

$$\delta P_1^+ \leq 0 \qquad \text{(B-20)}$$

for all admissible control variations δk and δw.

A) Inlet temperature control only (i.e., $w(t) = 1$ and $\delta w(t) = 0$). In this case (B-20) becomes from (B-19)

$$\delta P_1^+ = \int_0^1 \frac{\partial \overline{H}}{\partial k}\Big|_{k^+} \delta k dt \leq 0 \qquad \text{(B-21)}$$

where the boundary hamiltonian $\overline{H}$ is defined as in Equation (6-13) by

$$\overline{H} = \int_0^1 Hdz \qquad \text{(B-22)}$$

The condition (B-21) then implies

$$\left.\frac{\partial \bar{H}}{\partial k}\right|_{k^+} \begin{cases} = 0 \text{ whenever } k_* < k^+(t) < k^* \\ \geq 0 \text{ when } k^+(t) = k^* \\ \leq 0 \text{ when } k^+(t) = k_* \end{cases} \tag{B-23}$$

The conditions of (B-23) are identical to those defined by (6-14) - (6-16).

B) Inlet temperature and inlet flow rate control.

In this case (B-20) can be written as

$$\delta P_1^+ = \int_0^1 \left.\frac{\partial \bar{H}}{\partial k}\right|_{k^+} \delta k dt + \int_0^1 \left.\frac{\partial \bar{H}}{\partial w}\right|_{w^+} \delta w dt \leq 0 \tag{B-24}$$

where the boundary hamiltonian $\bar{H}$ now can be defined as in Equation (8-16) by

$$\bar{H} = \int_0^1 H dz + [x_1(t) - x_0(t)]\, w(t) - \kappa\left[\int_0^1 w(t)dt - 1\right] \tag{B-25}$$

The necessary condition for optimality (B-24) then implies:

$$\left.\frac{\partial \bar{H}}{\partial k}\right|_{k^+} \begin{cases} = 0 \text{ when } k_* < k^+(t) < k^* \\ \geq 0 \text{ when } k^+(t) = k^* \\ \leq 0 \text{ when } k^+(t) = k_* \end{cases} \tag{B-26}$$

and

$$\left.\frac{\partial \bar{H}}{\partial w}\right|_{w^+} \begin{cases} = 0 \text{ when } w_* < w^+(t) < w^* \\ \geq 0 \text{ when } w^+(t) = w^* \\ \leq 0 \text{ when } w^+(t) = w_* \end{cases} \tag{B-27}$$

The conditions (B-26) and (B-27) are identical to those given by (8-17) and (8-18).

APPENDIX C

CONVEXITY OF $\bar{H}$ WITH RESPECT TO k IN PROBLEM Π_0

From Equations (4-4) and (4-11) follows:

$$\frac{\partial \lambda(1-x)}{\partial z} = - \mu k r (1-x)^r \psi \tag{C-1}$$

Assuming continuity of $x_0(t)$, $k(t)$ and $\psi_0(z)$ guarantees the smoothness of $\mu(z,t)$ for $z \in [o,1]$, $t \in [o,1]$ and from (4-4), (4-12) and (C-1) follows then:

$$\frac{\partial}{\partial z}(\mu_t) = \frac{\partial}{\partial t}(\mu_z) = \mu_z k (1-x)^r \tag{C-2}$$

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

From (C-2) and (4-13) follows:

$$\mu_z = 0 \quad \text{for all } t \in [o,1] \quad \text{for all } z \in [o,1] \tag{C-3}$$

Hence

$$\mu_t = \mu_t\Big|_{z=1} = - K(k)(1-x(1,t)) + \mu(1,t)\, k(1-x(1,t))^r \qquad (C\text{-}4)$$

and from this follows that $\mu(z,t)$ is strictly positive for all $t \in [o,1)$ and zero at $t = 1$, unless $x(1,t) = 1$. Since $x(1,t) = 1$ requires $x_o(t) = 1$ from (4-4), this possibility can be excluded.

From (4-11) and (4-13) follows then also that λ remains strictly positive over the whole z x t domain.

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

$$\frac{\partial^2 \bar{H}}{\partial k^2} = \int_o^1 p(p-1)\, \lambda\, \frac{K(k)}{k^2}\, (1-x)\psi\, dz \qquad (C\text{-}5)$$

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

APPENDIX D

PROOF OF PROPERTY 2 OF PROBLEM $\prod_0$

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

Applying Pontryagin's maximum principle to the lumped parameter system (4-16) to (4-20), (4-26) and (4-27), with the hamiltonian H_ℓ defined by Equation (4-25), leads to the following necessary conditions for optimality:

$$\frac{\partial H_\ell}{\partial k} = 0 \quad \text{on } S \tag{D-1}$$

$$\frac{dH_\ell}{dt} = 0 \quad \text{for all } t \in [o,1] \tag{D-2}$$

and

$$\frac{d}{dt}\left(k \frac{\partial H_\ell}{\partial k}\right) = 0 \quad \text{on } S \tag{D-3}$$

where S is the region over which the optimal control is unconstrained. It is clear that all derivatives are evaluated at a Pontryagin policy. The derivation of the proof is then achieved in the following steps:

1. From (4-20), (4-25) and (D-2) follows:

$$\frac{df}{dt} = \frac{d}{dt}\left(\frac{\gamma k}{rK}\left(1 - \exp(-rK\phi)\right)\right) \quad \text{for all } t \in [o,1] \tag{D-4}$$

2. Substituting (D-4) into (D-3) gives:

$$p \frac{d}{dt} (K\phi \exp(-K\phi)) + (p-1) \frac{df}{dt} - p \frac{d}{dt} (\frac{\gamma k}{K} K\phi \exp(-rK\phi)) = 0$$

on S (D-5)

Before working out the time derivatives of the terms in (D-5), we first derive the following expressions:

a) From (4-19) we obtain

$$\frac{df}{dt} = \exp(-K\phi) \frac{dK\phi}{dt} \quad \text{for all } t \in [o,1] \tag{D-6}$$

b) Since $K = Ak^p$ we have

$$\frac{d}{dt} (\frac{k}{K}) = - \frac{p-1}{p} \frac{k}{K} \frac{1}{K\phi} (\frac{dK\phi}{dt} - K \frac{d\phi}{dt}) \tag{D-7}$$

From (D-7), (4-17), (4-26) and (D-1) it follows that

$$\frac{d}{dt} (\frac{\gamma k}{K}) = - \frac{p-1}{p} \frac{\gamma k}{K} \frac{1}{K\phi} \frac{dK\phi}{dt} \quad \text{on S} \tag{D-8}$$

3. Using (D-6) and (D-8), the expression (D-5) becomes

$$[2p - 1 - pK\phi + \frac{\gamma k}{K} \exp((1-r)K\phi)(prK\phi-1)] \frac{df}{dt}$$

$$= 0 \quad \text{on S} \tag{D-9}$$

4. Either df/dt or the bracketed term in (D-9) equals zero.

If df/dt = 0, the property holds.

If $df/dt \neq 0$ we must have:

$$[2p - 1 - pK\phi + \frac{\gamma k}{K} \exp((1-r)K\phi)(prK\phi-1)] = 0 \quad \text{on } S \qquad (D-10)$$

and all time derivatives of the bracketed term are also zero.

Multiplying (D-10) with $\exp(-K\phi)$ and adding the expression for $kr \frac{\partial H_\ell}{\partial k}$ results in

$$(2p - 1 - (1-r)pK\phi) \exp(-K\phi) - (p-1) \frac{\gamma k}{K} (\exp(-rK\phi) - 1)$$

$$- \frac{\gamma k}{K} \exp(-rK\phi) = 0 \quad \text{on } S \qquad (D-11)$$

Since then also the time derivative of (D-11) remains zero on S, we obtain by using (D-4) and (D-6):

$$(-3p + 1 + 2rp - r + (1-r)pK\phi) \frac{df}{dt} = \frac{d}{dt} (\frac{\gamma k}{K} \exp(-rK\phi)) \quad \text{on } S \qquad (D-12)$$

This expression (D-12) is the crucial one in eliminating terms involving γ in the time derivatives of (D-10). Using (D-4), (D-6) and (D-12), the first time derivative of (D-10), after first multiplying with $\exp(-K\phi)$, becomes:

$$[-3p + 1 + pK\phi - (1-prK\phi)(-3p + 1 + 2rp - r + (1-r)pK\phi)$$

$$+ pr \frac{\gamma k}{K} \exp((1-r)K\phi)] \frac{df}{dt} = 0 \quad \text{on } S \qquad (D-13)$$

Since we assumed that $df/dt \neq 0$, we can divide (D-13) by df/dt, and after multiplying the equation by $\exp(-K\phi)$, the next time derivative

becomes after rearranging

$$[p^2r(r-1)(K\phi)^2 + (p^2r(5r-6) + pr(2r-1))K\phi$$

$$- p^2r(4r-6) + pr(2r-5) + r]\frac{df}{dt} = 0 \quad \text{on } S \qquad \text{(D-14)}$$

Dividing again by df/dt leaves us with a polynomial in $K\phi$ which through further differentiation implies

$$\frac{dK\phi}{dt} = 0 \quad \text{on } S \qquad \text{(D-15)}$$

From (D-6) we see that (D-15) also implies

$$\frac{df}{dt} = 0 \quad \text{on } S \qquad \text{(D-16)}$$

Q.E.D.

APPENDIX E

CONVEXITY OF $\bar{H}$ WITH RESPECT TO k IN PROBLEM $\left[\ \right]_e$

We assume $e < 1$.

Since the $s_1 \times s_2$ domain is the only region of interest, we consider the adjoint equations as given by (4-65) and (4-66) with terminal and boundary conditions:

$$\lambda(s_{1f}, s_2) = 1 \ ; \ \mu(s_1, s_{2f}) = 0 \tag{E-1}$$

From (4-65), (4-66) and (E-1) it follows that $\lambda(s_1, s_2)$ and $\mu(s_1, s_2)$ are continuous and

$$\lambda(s_1, s_{2f}) > 0 \ ; \ \mu(s_{1f}, s_2) \geq 0 \tag{E-2}$$

Because of the continuity of λ it follows from (E-1) that when λ is negative at a point A inside the $s_1 \times s_2$ domain (Figure E-1), then there exists a point B, on the s_1 characteristic through A, where $\lambda(s_{1B}, s_{2A}) = 0$ with $s_{1A} < s_{1B} < s_{1f}$.

In order to prove that $\lambda(s_1, s_2)$ is strictly positive for all $s_1 \in [o, s_{1f}]$, $s_2 \in [o, s_{2f}]$, it is sufficient to prove that λ cannot become zero inside the $s_1 \times s_2$ domain.

The proof then proceeds in the following steps

1°) Supposing that λ becomes zero at some point inside the

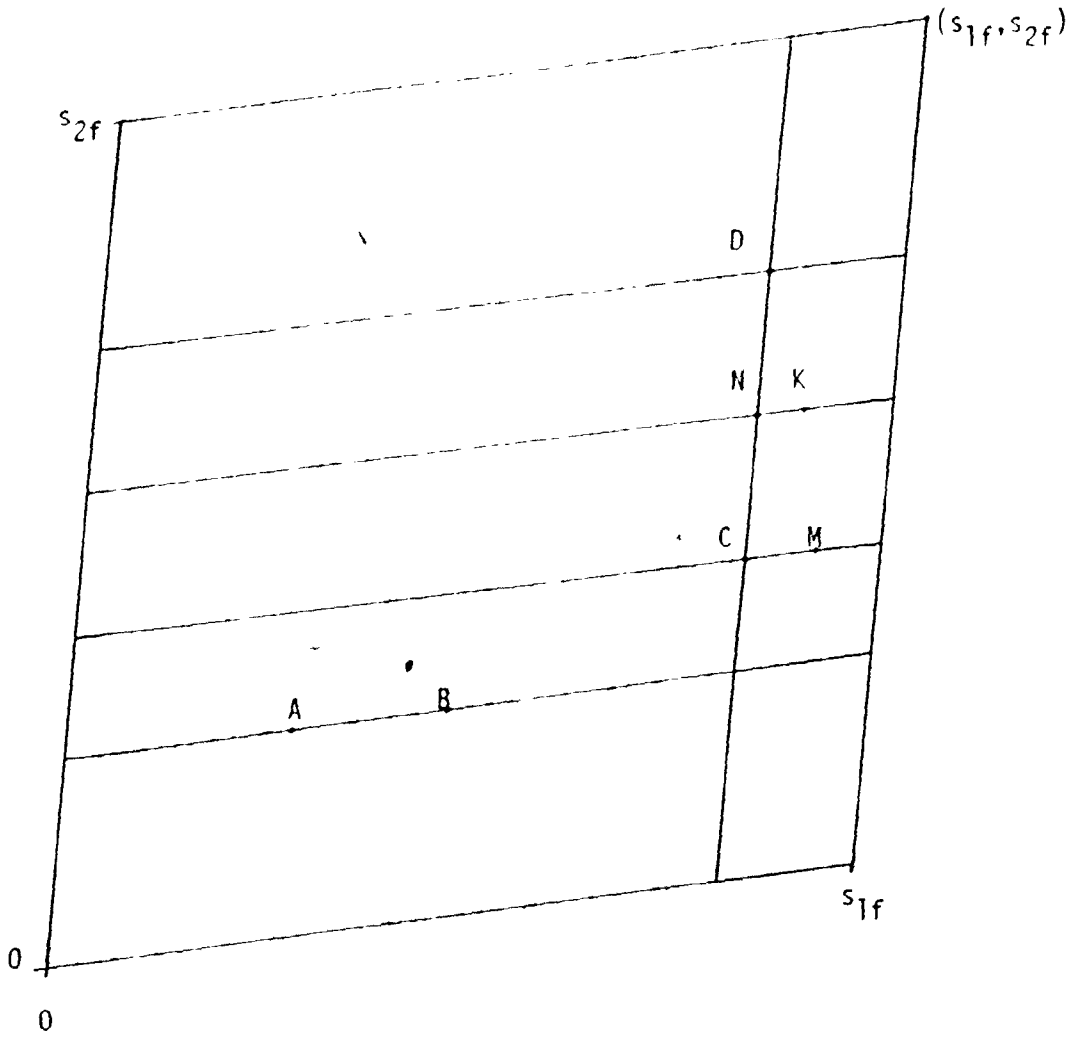

Figure E-1: Characteristic domain for Problem Π_e.

$s_1 \times s_2$ domain, then there exists a point $C(s_{1C},s_{2C})$(not necessarily unique) which lies closest to the s_2 characteristic at s_{1f}*. From (4-65) and (E-1) it follows then that $s_{1C} < s_{1f}$.

2°) $\mu(s_{1C},s_{2C}) = 0$.

Indeed, $\mu(s_{1C},s_{2C}) > 0$ would imply from (4-65) that λ becomes negative in the open interval (s_{1C},s_{1f}) on the s_1 characteristic through C. Hence there would exist a point $M(s_{1M},s_{2C})$ with $s_{1M} > s_{1C}$ where $\lambda(s_{1M},s_{2C}) = 0$ and this would contradict 1°).

Similarly $\mu(s_{1C},s_{2C}) < 0$ would imply from (4-66) and (E-1) that there exists a point $N(s_{1C},s_{2N})$ where $\lambda(s_{1C},s_{2N}) < 0$ with $s_{2N} > s_{2C}$. In fact λ would need to remain negative over a finite interval on the s_2 characteristic through C in order for μ to reach zero at (s_{1C}, s_{2f}). This however, would mean that there is a point $K(s_{1K},s_{2N})$ with $s_{1K} > s_{1C}$ where $\lambda(s_{1K},s_{2N}) = 0$ and this again would contradict 1°).

3°) On the s_2 characteristic through C, let D be the point closest to the terminal s_1 characteristic where $\lambda(s_{1D},s_{2D}) = \mu(s_{1D},s_{2D}) = 0$. From (E-2) follows $s_{2D} < s_{2f}$.

4°) From (4-65), (4-66), (E-1), (E-2), 1°), 2°) and 3°) it follows by contradiction that either $\lambda(s_{1D},s_2) = \mu(s_{1D},s_2) = 0$ or $\lambda(s_{1D},s_2) > 0$ and $\mu(s_{1D},s_2) \geq 0$ for all $s_2 \in [0,s_{2D})$; $\lambda(s_{1D},s_2) > 0$ and $\mu(s_{1D},s_2) \geq 0$ for all $s_2 \in (s_{2D},s_{2f}]$.

5°) From 4°) it is obvious that along the s_2 characteristic

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*It is most convenient to measure distances along the characteristic lines.

through D, the functions λ and μ reach a local minimum with respect to s_2 at D.

6°) The control $k(s_1,s_2)$ is positive over a finite open interval $(s_{2D}, s_{2D} + \eta)$ along the s_2 characteristic through D ($\eta > 0$). Indeed, it follows from (4-65) that $k = 0$ over that interval would result in a contradiction to 1°).

7°) $\mu(s_{1D},s_2) > 0$ for all $s_2 \in (s_{2D},s_{2D} + \eta)$. Indeed from 6°) and (4-66) it follows that $\mu \leq 0$ at any point of that interval would result in a contradiction to 4°).

8°) Since the initial condition $x_0(t)$ and the control $k(t)$ are piecewise continuous functions, it follows from (4-65) and (4-66), that in the interval $[s_{2D},s_{2D} + \eta)$ along the s_2 characteristic through D, both λ and μ are smooth functions of s_2 and hence differentiable. A necessary condition for having a local minimum for λ and μ at the point D is that the first nonzero right-hand derivative of λ and μ with respect to s_2 be positive.

9°) With $\lambda = \mu = 0$ at D, it follows from (4-66) that $d\mu/ds_2 = 0$.

Further differentiation of (4-66) with respect to s_2, up to the point where one of the derivatives of λ or μ becomes nonzero for the first time, leads to

$$\frac{d^{n+1}\mu}{ds_2^{n+1}} = - \frac{\partial^n \lambda}{\partial s_2^n} K(1-x) \qquad \text{(E-3)}$$

It is clear that all derivatives are right-hand derivatives of λ and μ with respect to s_2 at the point D.

Since in order to reach a local minimum at D, the first nonzero derivative has to be positive, Equation (E-3) cannot be satisfied for any finite value of n.

From the Taylor Theorem, it follows then that λ and μ remain zero in a neighbourhood of the point D in the interval $[s_{2D}, s_{2D} + \eta)$. This however, is in contradiction to 4°) and 7°) and therefore, the existence of any point D in the $s_1 \times s_2$ domain where λ becomes zero can be excluded.

10°) The expression for the second derivative of $\bar{H}$ with respect to k is identical to (C-5) and since again all factors in the integrand are positive for $k > 0$, $p > 1$ and $x_o(t) < 1$, $\bar{H}$ is a strictly convex function of k. Q.E.D.