DISSERTATION ABSTRACT

The quasi-steady state optimization of a single tubular fixed bed chemical reactor with a slowly decaying catalyst is considered. The optimal choice of temperature $T(z,t)$ distributed in both the space of the reactor and in chronological time is sought so as to maximize the total amount of reaction in a fixed given period of time. A single irreversible reaction is considered with a rate expressible as a product of separate functions of temperature, activity and conversion. The rate of catalyst decay is also a product of separate functions of temperature and activity but independent of conversion. Upper and lower bounds are placed on the permitted temperature. Theoretical characterization of the optimal policy is obtained using Sirazetdinov and Degtyarev's maximum principle derived for first-order partial differential equations and the influence of the ratio of reaction activation energy to catalyst deactivation energy on the derived optimal policy is indicated. Numerical calculations are presented to illustrate the optimal policies.

OPTIMIZATION BY DISTRIBUTED CONTROL OF REACTORS WITH DECAYING CATALYST

The contribution of chemical engineering to the industrial scale development of processes in the chemical and allied industries was initially attributable to the improved understanding it gave to the transport processes - fluid flow, heat transfer and mass transfer - and to the development of design principles for the unit operations and their control, nearly all of which are concerned with the physical separation of complex mixtures into their components.

With a fair degree of success achieved in the physical separation processes, interest has moved very much towards the design and control of the reactor and of more industrial concern : the catalytic reactor.

Chemical manufacture has become more demanding with a high proportion of the economic rewards to be obtained in the production of sophisticated chemicals. Profit margins have narrowed too, giving a far greater economic incentive to obtain the highest possible yield from raw materials and reactor design and control has therefore become a vital ingredient of the work of the chemical engineer.

The phenomenon of irreversible catalyst decay is very common in the catalytic chemical reactor and the number of commercial processes in which catalyst decay is an important factor is legion. For this reason and since temperature constitutes a most important operating variable of such reactors there has been much recent interest in the optimization of catalytic decaying reactors with both uniform and non-uniform temperature profiles varying in time.

The problem of optimally choosing the temperature $T(z,t)$, as a function of time t and position z in the reactor, so as to maximize the total yield of product over a fixed time period for a reaction-deactivation system with a slow decaying catalyst has been formulated by a number of authors but as yet no analytical solutions are available.

The significant feature of the present study is that using basically Sirazetdinov and Degtyarev's maximum principle formulation as the mathematical tool, for a tubular fixed-bed reactor and a quasi-steady state reaction-deactivation system, analytical expressions for the optimizing policies are obtained and characteristics of the optimal temperature controls identified.

Results of this approach are that the strong influence of the ratio of reaction activation energy to catalyst deactivation energy on the derived optimal policy is indicated and that properties of the optimal controls are used to reduce the computational dimensionality in synthesizing the control policies.

OPTIMIZATION

BY

DISTRIBUTED CONTROL OF REACTORS

WITH

DECAYING CATALYST

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by

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SCOPE AND CONTENTS:

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

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A single irreversible reaction is considered with a rate expressible as a product of separate functions of temperature, activity and conversion. The rate of catalyst decay is also a product of separate functions of temperature and activity but independent of conversion. Upper and lower bounds are placed on the permitted temperature. Theoretical characterization of the optimal policy is obtained using Sirazetdinov and Degtyarev's maximum principle derived for first-order partial differential equations and the influence of the ratio of reaction activation energy to catalyst deactivation energy on the derived optimal policy is indicated.

Numerical calculations are presented to illustrate the optimal policies.

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CHAPTER I

INTRODUCTION

Heterogeneous chemical reactions, where the catalyst condition is sensitive to any integrated effect or past history of the operating conditions, are common industrial problems in both fixed and moving bed reactors.

For such processes the catalyst activity decreases in chronological time under the effect of the operational conditions used but the rate of decay may be influenced by variations in the operating variables.

Since both the instantaneous reaction and catalyst decay rates depend upon the reactor temperature, it often constitutes the most important operating variable available for the control of such reactors.

There has been much recent interest in the optimization of reactors with both uniform and non-uniform temperature profiles varying in time and particular aspects of the research done in this field are discussed in section 2.3 of Chapter 2.

For a tubular fixed-bed reactor the current temperature profile in the reactor influences the whole future of the reaction by leaving its imprint on the catalyst activity profile. The problem of optimally choosing the temperature $T(z,t)$, as a function of time and position in the reactor, so as to maximize the total yield of product over a fixed time period has been formulated for the quasi-steady state reaction-deactivation process by Volin and Ostrovskii (1964, 1965_b), Jackson (1965, 1966, 1967) and recently by Ogunye and Ray (1969_a), but as yet no analytical solutions are available.

The maximum principle of Rozonoer (1959) or Pontryagin et al. (1962) is not applicable to a problem of this type with two independent variables z and t and this is discussed in sections 2.1 and 2.2 of Chapter 2.

Although an analogous principle can be found [Jackson (1966)] it has not proved possible to obtain the optimum policy directly by using it as a necessary condition. Ogunye and Ray (1969_a) also gave a weak form of a maximum principle for this case but as yet no investigation of the form of the optimizing policy for this problem has been reported other than computationally by Jackson (1965, 1967) who considered a reversible exothermic reaction.

That is, no direct analog of the analytical characterization of optimal policies as obtained for uniform temperature reactors, as discussed in section 2.3 of Chapter 2, is available.

The significant feature of the present study is that using basically Sirazetdinov and Degtyarev's (1967) maximum principle formulation, for the quasi-steady state reaction-deactivation process, analytical expressions for the optimizing policies are obtained and characteristics of the optimal controls identified.

Results of this approach are that the strong influence of the ratio of reaction activation energy to catalyst deactivation energy on the derived optimal policy is indicated and that properties of the optimal controls are used to reduce the computational dimensionality in synthesizing the control policies.

Chapter 3 discusses in detail the problem to be considered and the theory associated with the solution of such optimization problem is fully exposed in Chapter 4.

Chapter 5 represents the core of the thesis since properties of the

optimizing policies are stated and proved there.

Chapter 6 serves to illustrate the control policies recognized in the earlier chapter.

Finally Chapter 7 summarizes the results and conclusions obtained throughout the thesis.

CHAPTER 2

LITERATURE SURVEY

2.1 Optimal Control Theory and Lumped Parameter Systems

Contributions to the theory of optimal control have been concerned primarily with processes whose dynamic behaviour can be adequately described by a set of ordinary differential equations. These systems are referred to as lumped parameter systems.

The two theoretical approaches to the control optimization problem for such systems have been Bellman's (1957) dynamic programming method which is based on his principle of optimality and Rozonoer (1959) or Pontryagin's (1962) maximum principle which can be viewed as an extension and application of the classical calculus of variations to the optimal control problem.

The advantages and shortcomings of each method have been broadly discussed elsewhere [Roberts (1964), Pontryagin et al. (1962)]. It is worthwhile mentioning, however, that a major advantage of the maximum principle as well as other variational techniques, is that many characteristics of the optimum path may be determined without solving the entire problem.

2.2 Optimal Control Theory and Distributed Parameter Systems

While many physical systems have a spatial energy distribution sufficiently aggregated during the course of motion described by ordinary differential equations, there are systems for which energy relationships are important, not only as a function of time, but, in addition, as functions of one or more spatial variables.

These systems are called distributed parameter systems and are most naturally described by sets of partial differential equations, integral equations or integro-differential equations.

However, optimal control problems for these systems cannot be solved directly with the aid of Rozonoer (1959) or Pontryagin's (1962) maximum principle developed for lumped parameter systems.

Extension and generalization of the maximum principle to distributed parameter systems started only recently.

Most of the earlier work in this area has been carried out in the Soviet Union and a comprehensive survey of soviet publications on optimal control theory and its practical applications to such systems has been given by Butkovskii, Egorov and Lurie (1968).

A brief review is given below of the most important works pertaining to the establishment of a maximum principle as a necessary condition for optimality of distributed parameter systems described by partial differential equations.

2.2.1. Partial Differential Equations

One of the earliest and most persistent investigators of optimal control of distributed parameter systems was Butkovskii. His earlier publications attempted simply to define certain types of control problems that might arise. Butkovskii with Lerner subsequently considered the optimal control of a class of systems described by a set of non-linear integral equations, which result, in general, from the solution of partial differential equations. Butkovskii derived a maximum principle (in the sense of Pontryagin) embodying the necessary conditions for optimality of such systems. However, his results require before-

hand the explicit solution of the system equations, thus restricting the results to linear systems. An account of this work may be found in the recent book of Butkovskii (1969). This deficiency was removed by Katz (1964) who formulated a general maximum principle which could be applied to first-order hyperbolic systems and parabolic systems, as well as lumped parameter systems, and did not depend on the a priori representation of the system by integral equations. The generality of this functional analysis approach leads to some practical difficulty in implementation, because the adjoint operator must be constructed for each specific case.

At about the same time Egorov (1964, 1965, 1966, 1967) treated the optimal distributed control problem of a process described by second-order parabolic, hyperbolic and elliptic quasilinear partial differential equations. He extended Rozonoer's variational approach (1959) and obtained a maximum principle. These necessary conditions for optimality were shown to be also sufficient when the process is linear.

A comprehensive look at many properties of distributed parameter systems was given by Wang (1964) who introduced the concept of controllability and observability and derived necessary conditions similar to those of Katz (1964) and Egorov (1964) based on dynamic programming. His results are difficult to use since he obtains an implicit expression for the optimal control function in the form of a functional non-linear partial differential equation.

Sirazetdinov (1964) studied the optimal control of processes governed by a quasilinear first-order partial differential equation with $n^0 + 1$ independent variables $\underset{\sim}{z}$ and t but only one dependent variable $\phi^0(\underset{\sim}{z},t)$,

$$\frac{\partial \phi^0}{\partial t} + \sum_{j=1}^{n^0} a_j^0 \left(\underset{\sim}{z},t,\phi^0,\underset{\sim}{u}^0\right) \cdot \frac{\partial \phi^0}{\partial z_j} = f^0\left(\underset{\sim}{z},t,\phi^0,\underset{\sim}{u}^0\right) \qquad (2\text{-}1)$$

He derived a maximum principle as a necessary condition for optimality for cases in which the control functions are distributed both in time and space or only in time or space domain of the system. This maximum principle is also shown to be a sufficient condition for optimality of linear processes.

Jackson (1966) studied optimization problems where the system is described by two first-order partial differential equations but for the general case where the integral to be extremized is taken around a closed curve in the plane of the independent variables, and that this general closed curve includes finite straight segments parallel to the characteristic lines of the differential equations.

Variational theory and its extension were used by Jackson (1966) in this two-part work to show that a necessary condition for the control vector $\underset{\sim}{u}$ to maximize the integral around such a curve could be framed up as "the requirement that the control vector $\underset{\sim}{u}$ be chosen at each point of the domain such as to maximize a certain Hamiltonian function of the control vector": a maximum principle picture. However, these conclusions were derived only for the unconstrained control vector considered in that study.

In his dissertation Chang (1967) considered the optimal control of a system of simultaneous first-order partial differential equations in two independent variables z and t but for n' dependent variables $\underset{\sim}{\phi}(z,t)$ and obtained a maximum principle. That is for system of the form,

$$\frac{\partial \Phi_i}{\partial t} + a_i' (z,t,\underset{\sim}{u}) \cdot \frac{\partial \Phi_i}{\partial z} = f_i(z,t,\underset{\sim}{\phi},\underset{\sim}{u}) \qquad (2\text{-}2)$$

with $i = 1, \ldots, n'$.

The proof of the maximum principle lies essentially in,

i - the derivation of a formula for the incremental change of the function arguments corresponding to an arbitrary but admissible variation in the control vector $\underset{\sim}{u}$,

ii - the estimate of the second-order increments of the functions involved,

iii - the establishment of the theorem through proof by contradiction.

The method closely follows that of Rozonoer (1959) for a system of ordinary differential equations and that of Sirazetdinov (1964).

An independent work by Degtyarev and Sirazetdinov (1967) proved a maximum principle to be a necessary condition for the control optimization of a one-dimensional distributed process described by a set of simultaneous quasi-linear first-order partial differential equations of the following type,

$$\frac{\partial \Phi_i}{\partial t} + \sum_{j=1}^{n'} a''_{ij}(z,t,\underset{\sim}{\Phi}) \cdot \frac{\partial \Phi_j}{\partial z} = f_i(z,t,\underset{\sim}{\Phi},\underset{\sim}{u}) \qquad (2\text{-}3)$$

with $i=1,\ldots,n'$.

The proof of the maximum principle follows essentially the same basic steps cited earlier. In both approaches the control vector $\underset{\sim}{u}(z,t)$ is sought in the class of piecewise-continuous functions with a finite number of lines of discontinuity and may lie in a closed or open region U. The maximum principle established there is shown in both studies to be also a sufficient condition for optimality when system (2-3) is linear with a linear functional to be extremized.

A theoretical extension of Sirazetdinov's (1964) work has also been given by Tarassov (1968) and a maximum principle formulated for the system,

$$\frac{\partial \phi_i}{\partial t} + \sum_{j=1}^{n^o} a'_{ij}(\underset{\sim}{z},t,\underset{\sim}{u}^o) \cdot \frac{\partial \phi'_i}{\partial z_j} = f'_i(\underset{\sim}{z},t,\underset{\sim}{\phi}',\underset{\sim}{u}^o) \qquad (2\text{-}4)$$

with i=1,...,n', and constitutes a generalization of system (2-2).

The works noted above represent attempts to formulate a general maximum principle as a necessary condition for optimality of systems described by partial differential equations.

2.3. Optimal Operation of Reactors with Decaying Catalyst

2.3.1. Single Reactor with Uniform Temperature Profile

The problem of determining the optimum variations of uniformly distributed temperature with time in a single batch reactor (BSTR) and flow reactors of the CSTR and PFTR type during the life of the catalyst has been treated by Szepe (1966) using the Bolza form of the calculus of variations. The following types of rate equations were considered,

$$\text{rate of reaction} = K[T] \cdot F[X] \cdot \psi \qquad (2\text{-}5)$$

$$\text{rate of deactivation} = - k[T] \cdot g[\psi] \qquad (2\text{-}6)$$

with $g[\psi] = \psi^m$, $F[X] = [1-X]^n$ and both $K[T]$ and $k[T]$ of the Arrhenius form. X refers to the conversion for an irreversible reaction, ψ to the relative catalyst activity and T to temperature. The final catalyst activity $\psi(t_f)$, as well as the total time t_f, was specified beforehand and the temperature was considered to lie between higher and lower limits T* and T_*. Analytical characterization of the optimal policies is obtained.

Chou, Ray and Aris (1967) also studied the uniform temperature tubular reactor control policy in time using the Euler-Lagrange equations of the calculus

of variations but failed to determine if the extremal policies thus identified were indeed optimal or not. Ogunye and Ray (1968) subsequently treated a similar problem for the tubular reactor using the maximum principle of Pontryagin et al. (1962) and showed that the simple optimal policies given by Chou, Ray and Aris (1967) were not optimal. The approach of Chou, Ray and Aris (1967) and Ogunye and Ray (1968) was to constrain the temperature at or below a specified temperature T* and the conversion at or above a specified X_*. The total time t_f was free to be chosen, subject to the constraints, so that the policy for irreversible reactions always ended at $T = T^*$ and $X = X_*$.

The most detailed treatment of a problem of this class for the tubular reactor is that of Crowe (1969) who, using the maximum principle of Pontryagin et al. (1962), also gave a comparison of the conclusions of the workers cited above and indicated the effect of the problem statement on the derived policy. He fixed the operating time period and placed upper and lower bounds, T* and T_*, on the permitted temperature, but imposed no other constraints on the problem.

Lee and Crowe (1969) also studied the influence of an arbitrary residence time distribution on the optimal policy derived for this problem.

In addition reversible reactions [Drouin (1969)], parallel reactions [Rowbottom (1970)] and consecutive reactions [Alexander (1970)] has also been studied when the deactivation rate is of the form (2-6) with $g[\psi] = \psi^m$.

The problem of catalyst decay where the deactivation rate is a function of the degree of reaction in the reactor, that is,

$$\text{rate of deactivation} = \phi\,[T,\psi,X] \tag{2-7}$$

has been recently investigated by Crowe and Lee (1970) for the case of an

irreversible reaction occurring in a batch reactor (BSTR). The effect of conversion on catalyst decay and its influence on the derived extremal policy are indicated and the results obtained are compared with Szepe and Levenspiel's (1968_a) observation.

A similar reaction-deactivation scheme but occurring in a CSTR has recently been studied and the inter-relation between the factorability of the function (2-7),

$$\phi\,[T,\psi,X] = -\,k[T]\,.\,g[\psi]\,.\,f[X] \qquad (2\text{-}8)$$

and the derived extremal policy is indicated [Crowe and Thérien (1971)].

2.3.2. Multiple Reactors with Uniform Temperature Profile

The optimization of reactors with decaying catalyst but for a series of tubular fixed-bed reactors with uniform temperature was first studied by Volin and Ostrovskii (1965_a). The problem was treated as a distributed parameter system and variational arguments were used to obtain necessary stationary conditions for an extremum, but no bounds were placed on the permitted temperature.

Crowe and Lee (1969) further examined this problem and retaining the use of Pontryagin's (1962) maximum principle extended the result of a previous study [Crowe (1969)] to several beds in series, each with uniform temperature and uniform catalyst activity. A single irreversible reaction with reaction and decay rates given respectively by (2-5) and (2-6) were considered and characteristics of the optimal policy identified. Upper and lower bounds were placed on the permitted temperature and the operating time period is fixed.

A general formulation for problems of this class has been given by Ogunye and Ray (1969_b) where a distributed maximum principle for multi-bed reactors is derived. Analytic identification of characteristics of the optimal policy is no longer available and gradient methods are used to synthesize the extremal control policies.

Extending their first study Volin, Ostrovskii with Finkelshtein (1971) very recently obtained necessary conditions for optimality in the form of a weak and strong distributed maximum principle.

2.3.3. Single Reactor with Non-Uniform Temperature Profile

When the problem is generalized by eliminating the assumption that the reactor is uniform in temperature, the temperature may become a function of position in the reactor, as well as time, and the maximum principle of Pontryagin et al. (1962) is no longer applicable.

Such an optimization problem has been first carried out by Volin and Ostrovskii (1964, 1965_b) who derived necessary stationary conditions for the optimal operation of a tubular chemical reactor based on calculus of variations. They considered the case where the temperature is distributed in both space and time but unconstrained. A steepest descent algorithm was proposed to solve the problem.

The problem was also considered by Jackson (1965, 1967). The object of this study was to develop a criterion of optimality based on a variational method which could provide the basis of a computational procedure to solve for the extremal temperature policy. An optimizing algorithm based on gradient in function space is derived and results of some preliminary computations for the case of a reversible exothermic reaction is reported.

The derivation of a weak form of a maximum principle which could treat a problem of this class has recently been given by Ogunye and Ray (1969_a). This result states that the Hamiltonian like function arising from such variational analysis be a maximum at boundaries and simply stationary for interior values of the optimal decision. Since no second-order necessary condition is considered in their derivation, the stationary condition alone does not guarantee that the Hamiltonian is a maximum for interior points of the decision function, and, this result is significantly weaker than the condition that the Hamiltonian takes its absolute maximum value when evaluated for the optimal decision function: a strong form of the maximum principle as derived by Rozonoer (1959) or Pontryagin et al. (1962) for lumped systems. An efficient computational algorithm is presented and several detailed numerical examples are worked out. No consideration is given to the analytical characterization of an optimal policy and the problem of best choosing the temperature $T(z,t)$ in both space and time is not treated.

CHAPTER 3

CATALYTIC REACTOR SYSTEM

3.1. Tubular Fixed-Bed Catalytic Reactor

A tubular fixed bed catalytic chemical reactor consists in its simplest form of a cylindrical tube packed with pellets of catalyst through which reactants are passed and converted into products in an amount depending upon the controlled parameters of the system. In general, industrial catalytic reactors use catalyst particles that are small compared to the overall geometry of the reactor itself, and therefore it has been customary to write continuum models for the interstitial fluid. The particle itself is considered as a continuum imbedded in a field of concentration and temperature, the particle being small enough so that it may be assumed the fields with which it interacts are uniform. The system as a whole has been described by non-linear partial differential equations of great complexity [Amundson (1970)].

However, when the analytical description of the process is not readily solvable another customary approach has been to consider the reaction system as a pseudo-homogeneous one where the equations are written as though the system did not contain the solid catalyst phase. This approach simplifies the equations describing the system, however not without a price, for the correspondence of the real and equivalent systems depends upon how completely the effects of the solid phase can be included in the equivalent homogeneous equations [Petersen (1965)].

Nevertheless, when the heat and mass transfer between the catalyst and the fluid phase is very rapid and when the reactor tube has enough catalyst

particles per unit volume that a continuum representation is adequate this simplification is reasonably justifiable.

The continuity equation in terms of molar units for a component i in some reactor element may be written,

$$\frac{\partial c_i}{\partial t'} + \nabla . c_i v + \nabla . J_i = R_i \qquad (3\text{-}1)$$

where c_i is the molar concentration of species i, v is the molar average velocity, J_i is the molar flux of species i relative to the molar average velocity and R_i is the molar rate of production of species i. When the density of the reacting fluid is nearly a constant for the range of operations considered,

$$\nabla . c_i v = v . \nabla c_i \qquad (3\text{-}2)$$

and if flow component is considered in the flow direction along the axis of the tubular reactor only,

$$v . \nabla c_i = v . \frac{\partial c_i}{\partial z'} \qquad (3\text{-}3)$$

Now when the axial diffusion is negligible and that no radial concentration gradient exists,

$$\nabla . J_i = 0 \qquad (3\text{-}4)$$

and finally (3-1) may be rewritten,

$$\frac{\partial c_i}{\partial t'} + v . \frac{\partial c_i}{\partial z'} = R_i \qquad (3\text{-}5)$$

For a single chemical reaction, the rate of reaction R_i may be expressed as a function of temperature $T(z',t')$, chemical conversion $X(z',t')$ and catalyst relative activity $\psi(z',t')$,

$$R_i = \Omega\,[T,X,\psi] \tag{3-6}$$

and (3-5) formulated,

$$\frac{\partial X}{\partial t'} + v \cdot \frac{\partial X}{\partial z'} = \Omega\,[T,X,\psi] \tag{3-7}$$

The pseudo-homogeneous rate of an irreversible chemical reaction $A \rightarrow B$ is expressed in this study as the product of separate functions each depending on only one of the state or decision variable, and,

$$\Omega\,[T,X,\psi] = K'[T] \cdot F[X] \cdot \psi \tag{3-8}$$

Weller (1956) has shown that this product of functions is compatible with much more complex forms of the rate of reaction and that in some cases it is a better representation. Therefore (3-7) may be written with (3-8),

$$\frac{\partial X}{\partial t'} + v \cdot \frac{\partial X}{\partial z'} = K'[T] \cdot F[X] \cdot \psi \tag{3-9}$$

z' is the distance along the bed, $z' \in [0,L]$ where L is the length of the bed, and t' is the chronological time, $t' \in [0,t_f]$, since start-up of the reactor with t_f representing the terminal reaction time.

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

$$K'[T] = K_o \cdot \exp\{- E_R/(R.T)\} \tag{3-10}$$

with K_o and R representing constants and E_R the reaction activation energy. The function $F[X(z',t')]$ is considered a continuous, generally non-linear monotonic decreasing function of conversion $X(z',t')$, or a constant, such that for,

$$o \leqslant X(z',t') \leqslant 1 \tag{3-11}$$

then

$$o \leqslant F[X(z',t')] \leqslant 1 \tag{3-12}$$

and $F[X]$ is twice continuously differentiable with respect to its argument. The relative effectiveness of the catalyst is measured by its relative activity $\psi(z',t')$ defined as,

$$\psi(z',t') = \frac{\text{rate of reaction using catalyst in a given condition}}{\text{rate using fresh catalyst, or catalyst in a reference state}} \tag{3-13}$$

Anderson (1968) recently stressed the importance of characterizing the relative catalyst activity in this manner since the combined effect of operating condition, type of contacting pattern and the kinetics itself are eliminated.

Natural spatial and time boundary conditions for equation (3-9) are

$$X(o,t') = X_o(t') \tag{3-14}$$

with

$$X(z',o) = X_1(z') \tag{3-15}$$

where $X_o(t')$ and $X_1(z')$ 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 plane considered $\tau = T^o \times Z^o = [o,t_f] \times [o,L]$, but with a finite number of discontinuities there.

However, when the space time (time required to process one void reactor volume) is small (minutes or seconds) compared to the average time of total decay of the catalyst (days or hours), the change in relative activity $\delta\psi(z',t')$ over a space time is very nearly negligible, and the quasi-steady state approximation is validated (Appendix F),

$$\frac{\partial X}{\partial t'} << v \cdot \frac{\partial X}{\partial z'} \tag{3-16}$$

then equation (3-9) may be written for the quasi-steady state reaction-deactivation process,

$$v \cdot \frac{\partial X}{\partial z'} = K'[T] \cdot F[X] \cdot \psi \tag{3-17}$$

with the natural boundary (3-14).

3.2. Catalyst Deactivation

While the process of catalyst deactivation is a complex phenomenon, nevertheless various general types of mechanisms contributing to deactivation can be identified and have been extensively mentioned in the literature. Loss in activity may be due to sintering, fouling or poisoning of the catalyst.

Sintering is often encountered in practice and is due to loss in activity through structural changes in the catalyst itself and is an irreversible process. It is mainly caused by unfavorable operating conditions. In particular, a high level of temperature may cause localized melting of the catalyst, hence a reduction of its active surface.

Fouling is a rather common problem in the hydrocarbon processing industry and is caused by side reactions which develop with the reactants and/or products formed by the main reaction. Carbonaceous compounds formed by these side reactions deposit and accumulate on the catalytic surface and block the diffusion of reactants into porous pellets.

Poisoning refers to a process where impurities in the feed of reactants to the reactor reduce the active surface by preferential adsorption or surface reaction.

3.2.1. Quantitative Characterization of Catalyst Decay

A multitude of cases relating quantitatively the degradation of a catalyst condition and number of models have been presented in the literature.

The unified interpretation of these studies offers two major difficulties and have been discussed by Szepe (1966):

- one consists in the way authors have expressed or defined the catalyst condition or activity,

- the second is that the functional form relating the catalyst condition has been often reported, mainly in the early literature, explicitly as a function of time on stream.

This latter observation is more serious since it is based on integral measures only, such as the outlet conversion of a reactor, and thus gives a descriptive image of the catalyst activity with time but averaged over the whole reactor. Local characterization of the catalyst condition may however be assured using functional forms relating the relative activity to the local concentration of adsorbed or deposited materials on the catalyst [Anderson and Whitehouse (1961)]. A number of equations for expressing the relative activity as a function of the concentration of the adsorbed or deposited species on a catalyst have been reported in the literature. The most recognized forms of decay have been linear, exponential or hyperbolic in form and experimental evidence of such results may be found in the works of Takeuchi et al. (1966) and Ozawa and Bischoff (1968).

A simple but theoretically acceptable and satisfactory form for the rate of deactivation has been shown by Szepe (1966) to be describable similarly to a chemical reaction rate expression and to be a function of the operating and catalyst condition,

$$\text{rate of deactivation} = - k'[T] \cdot f[X] \cdot g[\psi] \tag{3-18}$$

with the simplest possible but still admissible form,

$$\text{rate of deactivation} = - k'[T] \cdot g[\psi] \tag{3-19}$$

where $g[\psi]$ of the power form,

$$g[\psi] = \psi^m \tag{3-20}$$

and k'[T] of the Arrhenius form,

$$k'[T] = k_o \cdot \exp\{- E_c/(R.T)\} \qquad (3\text{-}21)$$

The pre-exponential factor k_o and R are constants and E_c the catalyst deactivation energy. The parameter m in (3-20) is called the deactivation order.

More complex deactivation processes may however exist for which expression (3-19) or even (3-18) may not be a true representation [Wheeler and Robell (1969)]. Nevertheless, these expressions may be a satisfactory first approximation to many such complex deactivation processes.

Szepe (1966) found that five different types of deactivation equations most currently referred to in the literature, including the linear, exponential and hyperbolic form and obtained on the basis of experiments, are all special cases of expression (3-19) with $g[\psi]$ given by (3-20).

An analysis of the published data by Szepe and Levenspiel (1968_b) shows that cracking catalyst deactivation can be well described by expression (3-19) with the power form (3-20) where m is usually close to 3. Levenspiel and Szepe (1971) have also shown that this kinetic form is consistent with and can be explained by the mechanism of progressive deposition of carbon at the mouth of catalyst pores.

A systematic experimental investigation of sintering on industrial catalyst by Schlaffer et al. (1957) and later by Maath and Mascou (1965) has shown, under all conditions studied, that the rate of decline in the catalyst active surface is most satisfactory described by a function of the power form such as (3-19) with (3-20). The parameter m averaged nearly a constant value of 4 when thermal sintering alone was considered and has been reported

by Schlaffer et al. for a silica-alumina catalyst. A value of m = 2 was proven satisfactory in the later study of Maath and Mascou on a platinum reforming catalyst.

Recognizing the importance of retaining in this study a simple but admissible functional form for catalyst deactivation, the rate of change of the catalyst relative activity is written,

$$\frac{\partial \psi}{\partial t'} = - k'[T] \cdot g[\psi] \tag{3-22}$$

where the function $g[\psi(z',t')]$ is considered a continuous, generally non-linear monotonic increasing function of relative activity $\psi(z',t')$, or a constant, such that for

$$0 \leqslant \psi(z',t') \leqslant 1 \tag{3-23}$$

then

$$0 \leqslant g[\psi(z',t')] \leqslant 1 \tag{3-24}$$

and is twice continuously differentiable with respect to its argument. The function $k'[T(z',t')]$ is assumed of the form (3-21) and is then a positive continuous strictly monotonic increasing and differentiable function of temperature $T(z',t')$.

A natural time boundary condition

$$\psi(z',0) = \psi_0(z') \tag{3-25}$$

where $\psi_0(z')$ is given and may in general be a piecewise-continuous function of z' and has a piecewise-continuous first derivative with respect to z' but with a finite number of discontinuities.

3.3. Formulation of the Optimization Problem

Defining for convenience the transformations,

$$z = z'/L \tag{3-26}$$

and,

$$t = t'/t_f \tag{3-27}$$

with

$$K[T] = t_f \cdot K'[T] \tag{3-28}$$

and

$$k[T] = t_f \cdot k'[T] \tag{3-29}$$

then the variables $z\varepsilon[o,1]$, $t\varepsilon[o,1]$, $K[T]$ and $k[T]$ have been made dimensionless. The unsteady state catalytic reactor system may then be written with $t_\Theta = (L/v)$,

$$\frac{\partial X}{\partial t} + \left(\frac{t_f}{t_\Theta}\right) \cdot \frac{\partial X}{\partial z} = K[T] \cdot F[X] \cdot \psi = \Omega \tag{3-30}$$

and the quasi-steady state system,

$$\left(\frac{t_f}{t_\Theta}\right) \cdot \frac{\partial X}{\partial z} = K[T] \cdot F[X] \cdot \psi = \Omega \tag{3-31}$$

with the rate of decay,

$$\frac{\partial \psi}{\partial t} = - k[T] \cdot g[\psi] = \phi \tag{3-32}$$

The corresponding initial and boundary conditions being,

$$X(o,t) = X_o(t) \tag{3-33}$$

$$X(z,o) = X_1(z) \tag{3-34}$$

$$\psi(z,o) = \psi_o(z) \tag{3-35}$$

3.3.1. The Control Alternative

The temperature sought is constrained by some upper and lower bounds, T^* and T_*, such that,

$$T_* \leqslant T(z,t) \leqslant T^* \tag{3-36}$$

which may be imposed from physical, legal or profit considerations. Since by assumption, K[T] and k[T] are both of Arrhenius form, from (3-10), (3-21), (3-28) and (3-29),

$$K[T] = A \cdot k^p[T] \tag{3-37}$$

with,

$$A = t_f \cdot K_o/(k_o \cdot t_f)^p \tag{3-38}$$

and p represents the ratio of reaction activation/energy to deactivation energy,

$$p = E_R/E_c \tag{3-39}$$

and since k[T] is a strictly monotonic increasing function of temperature T(z,t), the temperature is replaced more conveniently as a decision variable by k[T], that is corresponding to (3-36),

$$k_* \leqslant k[T] \leqslant k^* \tag{3-40}$$

where $k_* = k[T_*]$ with $k^* = k[T^*]$ from (3-21) and (3-29).

3.3.2. The Quasi-Steady State Problem

The precise statement of the optimization problem for the quasi-steady state reaction-deactivation process is as follows:

Given the system equations: (3-31) and (3-32).

Given the initial and boundary conditions: (3-33) and (3-35).

Given the control constraint: (3-40),

maximize the total amount of reaction from the reactor shown in Figure 3-1 over a fixed reaction time, by choosing the rate constant $k[T(z,t)]$, hence $T(z,t)$, at every instant $t\varepsilon[o,1]$ and any position $z\varepsilon[o,1]$ along the reactor length, that is,

$$J^{+} = \max_{k[T(z,t)]} J = \max_{k[T(z,t)]} \int_{o}^{1} \{X(1,t) - X_{o}(t)\} \cdot dt \qquad (3\text{-}41)$$

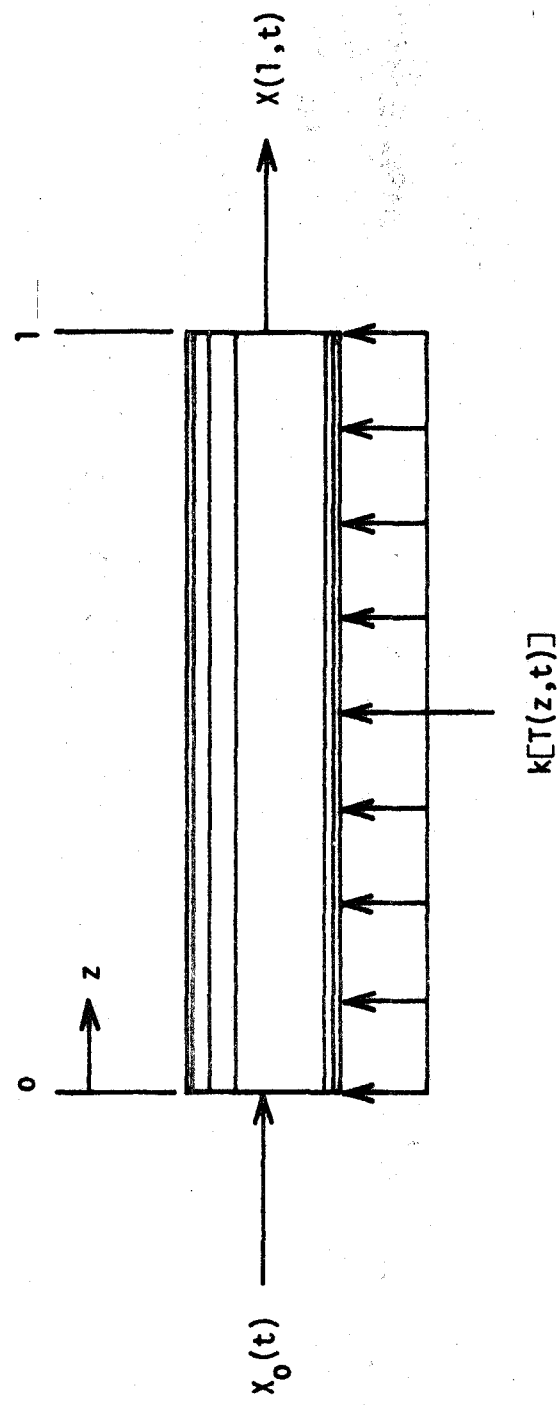

Figure 3-1. Single-Bed Reactor.

CHAPTER 4

OPTIMAL CONTROL THEORY

4.1. Formulation of a General Optimization Problem

Let a process take place in a bounded region τ,

$$\tau = T^o \times Z^o = [t_o, t_f] \times [z_o, z_f] \tag{4-1}$$

and let it be described by the following system of first-order partial differential equations,

$$\frac{\partial \Phi_i(z,t)}{\partial t} + \sum_{j=1}^{n'} a_{ij}(z,t) \frac{\partial \Phi_j(z,t)}{\partial z} = f_i(z,t,\underset{\sim}{\Phi}, \underset{\sim}{u}) \qquad i=1,\ldots,n' \tag{4-2}$$

where the n'-dimensional vector,

$$\Phi = \underset{\sim}{\Phi}(z,t) = \{\Phi_1(z,t),\ldots, \Phi_{n'}(z,t)\} \tag{4-3}$$

is the vector function describing the state of a process at any point $(z,t) \in \tau$. The coefficients $a_{ij}(z,t)$ are real and continuous functions of z and t and continuously differentiable with respect to them in τ. The n' x n' matrix of the coefficients is assumed to define system (4-2) as a totally hyperbolic system in the whole of τ (see Appendix A).

The r-dimensional vector,

$$\underset{\sim}{u} = \underset{\sim}{u}(z,t) = \{u_1(z,t),\ldots, u_r(z,t)\} \tag{4-4}$$

is the control vector distributed in z and t of τ.

The optimal control vector,

$$\underset{\sim}{u}^{+} = \underset{\sim}{u}^{+}(z,t) = \{u_1^{+}(z,t),\ldots, u_r^{+}(z,t)\} \tag{4-5}$$

belonging to a closed set U,

$$\underset{\sim}{u}_{*} \leqslant \underset{\sim}{u}^{+}(z,t) \leqslant \underset{\sim}{u}^{*} \tag{4-6}$$

will be sought in the class of arbitrary piecewise continuous controls, i.e., controls $\underset{\sim}{u}(z,t)$ which are continuous for all z,t under consideration, with the exception of only a finite number of lines of discontinuity in τ at which the controls $\underset{\sim}{u}(z,t)$ may have discontinuities of the first kind. Recalling that discontinuities of the first kind imply the existence of finite limits for the values of the controls at both sides of a line of discontinuity, controls satisfying the above conditions will be called admissible controls.

Each, generally non-linear, i^{th} component of the n-dimensional vector function,

$$\underset{\sim}{f} = \underset{\sim}{f}(z,t,\underset{\sim}{\phi},\underset{\sim}{u}) = \{f_1(z,t,\underset{\sim}{\phi},\underset{\sim}{u}),\ldots, f_{n'}(z,t,\underset{\sim}{\phi},\underset{\sim}{u})\} \tag{4-7}$$

is a twice continuously differentiable real function with respect to the control vector $\underset{\sim}{u}(z,t)$ and the state vector $\underset{\sim}{\phi}(z,t)$ in τ, and also a real, continuous function of the explicitly appearing independent variables z and t.

The initial and boundary conditions associated with system (4-2) are,

$$\phi_i(z,t_o) = \alpha_i(z) \qquad i=1,\ldots,n' \tag{4-8}$$

$$\phi_i(z_o,t) = \beta_i(t) \qquad i=1,\ldots,n' \tag{4-9}$$

where the i^{th} component of the vectors $\underset{\sim}{\alpha}$ and $\underset{\sim}{\beta}$ may in general be piecewise continuous functions of z and t and have piecewise continuous first derivatives with respect to z and t along their respective boundaries of τ. That is, the components $\alpha_i(z)$ and $\beta_i(t)$ are continuous functions and have continuous first derivatives with z and t respectively for all $z \in Z^o$ and all $t \in T^o$ under consideration, except for a finite set of points on Z^o and T^o, where $\alpha_i(z)$ and/or $\dfrac{d\,\alpha_i(z)}{dz}$ and $\beta_i(t)$ and/or $\dfrac{d\,\beta_i(t)}{dt}$ may have discontinuities of the first kind.

If an admissible control vector $\underset{\sim}{u}(z,t)$ is specified in the whole of τ, system (4-2) with the available initial conditions (4-8) and boundary conditions (4-9) may be shown to possess a uniquely determined solution vector $\underset{\sim}{\phi}(z,t)$ in the whole of τ (see Appendix A).

On the set of such solutions, the following functional is defined,

$$I = \int_{t_o}^{t_f}\int_{z_o}^{z_f} G_1[\underset{\sim}{\phi}(z,t),\underset{\sim}{u}(z,t)]\,dz\,dt + \int_{z_o}^{z_f} G_3[\underset{\sim}{\phi}(z,t_f)]\,dz + \int_{t_o}^{t_f} G_2'[\underset{\sim}{\phi}(z_o,t)]\,dt + \int_{t_o}^{t_f} G_2''[\underset{\sim}{\phi}(z_f,t)]\,dt \tag{4-10}$$

where G_1, G_2', G_2'' and G_3 are twice continuously differentiable real functions with respect to their arguments.

The optimal distributed control problem is then defined as:

"Find an admissible distributed control vector $\underset{\sim}{u}^{+}(z,t)$ that makes the functional I a minimum"

4.2. Formulation of a Maximum Principle

Introduce the following scalar function,

$$H(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}) = - G_1[\underset{\sim}{\phi},\underset{\sim}{u}] + \sum_{i=1}^{n'} \psi_i(z,t) \cdot f_i(z,t,\underset{\sim}{\phi},\underset{\sim}{u}) \tag{4-11}$$

where the costate variables $\psi_i(z,t)$ satisfy the set of equations,

$$\frac{\partial \psi_j(z,t)}{\partial t} + \sum_{i=1}^{n'} \frac{\partial\{a_{ij}(z,t).\psi_i(z,t)\}}{\partial z} = - \frac{\partial H(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u})}{\partial \Phi_j(z,t)} \qquad j=1,\ldots,n' \tag{4-12}$$

with the associated terminal and boundary conditions,

$$\psi_i(z,t_f) = - \frac{\partial G_3[\underset{\sim}{\phi}(z,t_f)]}{\partial \Phi_i(z,t_f)} \qquad i=1,\ldots,n' \tag{4-13}$$

and

$$\sum_{i=1}^{n'} a_{ij}(z_f,t) \cdot \psi_i(z_f,t) = - \frac{\partial G_2''[\underset{\sim}{\phi}(z_f,t)]}{\partial \Phi_j(z_f,t)} \qquad j=1,\ldots,n' \tag{4-14}$$

where the vector functions $\underset{\sim}{\phi}(z,t_f)$ and $\underset{\sim}{\phi}(z_f,t)$ are unspecified. Here, the vector functions $\underset{\sim}{\phi}(z,t)$ and $\underset{\sim}{\psi}(z,t)$ represent the solution of the boundary-value

problem defined by equations (4-2), (4-8), (4-9), (4-12), (4-13) and (4-14) corresponding to the specified admissible control vector $\underset{\sim}{u}(z,t)$ in τ.

The scalar function (4-11) plays a role similar to the Hamiltonian function of the maximum principle of Pontryagin et al. (1962). An admissible control vector $\underset{\sim}{u}^{+}(z,t) \in U$ is said to satisfy the maximum condition if:

$$H[z,t,\underset{\sim}{\phi}^{+}(z,t),\underset{\sim}{\psi}^{+}(z,t),\ \underset{\sim}{u}^{+}(z,t)]$$

$$= \underset{\underset{\sim}{u}(z,t) \in U}{\text{supremum}} \quad H[z,t,\underset{\sim}{\phi}^{+}(z,t),\ \underset{\sim}{\psi}^{+}(z,t),\ \underset{\sim}{u}(z,t)] \tag{4-15}$$

where $\underset{\sim}{\phi}^{+}(z,t)$ and $\underset{\sim}{\psi}^{+}(z,t)$ are the solutions of the boundary-value problem defined by equations (4-2), (4-8), (4-9), (4-12), (4-13) and (4-14) using control vector $\underset{\sim}{u}^{+}(z,t)$.

The necessary condition for an admissible control vector to be optimal in the whole of τ is given in the following theorem [Sirazetdinov and Degtyarev (1967)]:

> "If an admissible control vector $\underset{\sim}{u}(z,t)$ defined on τ is to yield a minimum of functional (4-10), it is necessary that the admissible control vector $\underset{\sim}{u}(z,t) \in U$ satisfy the maximum condition (4-15) everywhere in τ except possibly on a subset $\delta\tau^{o} \subset \tau$ whose measure is zero."

If both system (4-2) and functional (4-10) are linear, this theorem becomes a necessary and sufficient condition for optimality.

A detailed proof of the theorem is given in Appendix B.

4.3. A Global Maximum Condition

The maximum condition (4-15) expressed in the previously stated theorem may also be conveniently written,

$$H[z,t,\underset{\sim}{\phi}^+,\underset{\sim}{\psi}^+,\underset{\sim}{u}^+] \geq H[z,t,\underset{\sim}{\phi}^+,\underset{\sim}{\psi}^+,\underset{\sim}{u}] \tag{4-16}$$

for all $\underset{\sim}{u}(z,t) \in U$.

Since for fixed values of $\underset{\sim}{\phi}^+(z,t)$ and $\underset{\sim}{\psi}^+(z,t)$ at any chosen point $(z,t) \in \tau$ the function H becomes a function solely of the control vector $\underset{\sim}{u}(z,t)$, the maximum condition (4-16) instructs us unequivocally to take at that point $(z,t) \in \tau$ the greatest value of the function H globally with respect to <u>all</u> admissible control vectors $\underset{\sim}{u}(z,t) \in U$.

Thus the maximum condition (4-16) provides a necessary test which determines globally over <u>all</u> admissible control vectors $\underset{\sim}{u}(z,t) \in U$ whether or not any given control vector $\underset{\sim}{\bar{u}}(z,t) \in U$ is a candidate for optimality at a point $(z,t) \in \tau$. If the given control vector $\underset{\sim}{\bar{u}}(z,t)$ violates the maximum condition (4-16) there, one is assured that the control vector $\underset{\sim}{\bar{u}}(z,t)$ cannot be optimal at that point in τ.

On the other hand, the mere fact that a control vector $\underset{\sim}{\hat{u}}(z,t) \in U$ satisfies the maximum condition at that point is not enough to guarantee that $\underset{\sim}{\hat{u}}(z,t)$ is the optimal control vector.

The reason is that the maximum condition (4-15) or (4-16) resulting from the maximum principle formulation is a necessary condition for the optimality of a control vector $\underset{\sim}{\hat{u}}(z,t) \in U$ but is not, in general, a sufficient condition. Furthermore, the use of the maximum condition (4-15) or (4-16) in itself does not guarantee that the greatest value of the function H with respect

to all admissible control vector $\underset{\sim}{u}(z,t) \in U$ at a point $(z,t) \in \tau$ corresponds to a unique control vector $\hat{\underset{\sim}{u}}(z,t) \in U$.

For this reason, the set of control vectors $\hat{\underset{\sim}{u}}(z,t) \in U$ which satisfy the global maximum condition at a point $(z,t) \in \tau$ and are thus candidates for optimality will be referred to as the set of extremal control vectors,

$$\hat{U}(z,t) = \{\hat{u}_1(z,t),\ldots,\hat{u}_p(z,t)\} \tag{4-17}$$

If an optimal control vector $\underset{\sim}{u}^+(z,t)$ exists, then it belongs to the set of extremal control vectors $\hat{U}(z,t)$. Of course, more than one extremal control vector $\hat{\underset{\sim}{u}}(z,t)$ may be optimal, i.e., the optimal control vector $\underset{\sim}{u}^+(z,t)$ when it exists need not be unique. However, there may exist extremal control vectors $\hat{\underset{\sim}{u}}(z,t) \in \hat{U}(z,t)$ which are not optimal.

Thus in applying a maximum principle in order to deduce an optimal control vector $\underset{\sim}{u}^+(z,t) \in U$, one is faced with two major tasks:

i - establish that an optimal control vector $\underset{\sim}{u}^+(z,t) \in U$ exists.

ii - to find all extremal control vectors $\hat{\underset{\sim}{u}}(z,t) \in \hat{U}(z,t)$.

The first of these tasks requires knowledge of existence theorems for optimal control.

4.3.1. Existence of Optimal Control

Questions regarding the existence of optimal controls are complicated. Investigations and results pertaining to the existence of optimal controls for systems described by ordinary differential equations can be found in the works of Pontryagin et al. (1962), Roxin (1962), Markus and Lee (1961), Filippov (1963), Neustadt (1963), Cesari (1965), LaSalle (1960) and Halkin (1965).

Most of these references deal with the existence of optimal controls when the state enters linearly into the ordinary differential equations.

The most important works at present and pertaining to the existence of optimal controls in systems described by partial differential equations are undoubtedly due to Lions and his coworkers and to Cesari (1968). An account of this work may be found in the recent book of Lions (1968) and in the thesis of Bensoussan (1969).

Most of the available results at present use measure theory and the concept of measurable functions in the derivation of the results.

One "practical" shortcoming of these investigations is that they deal with the existence of optimal controls which are measurable functions. As Halkin (1964) has pointed out: "one must know measure theory in order to imagine a function which is not measurable". That is, continuous and piecewise continuous functions are measurable functions, however, there are measurable functions which are neither continuous nor piecewise continuous. The search for existence theorems for optimal controls which are specifically piecewise continuous is much more "practical" from an engineering point of view.

Such an investigation has been conducted by Halkin (1965) regarding the existence of piecewise continuous time-optimal controls for linear-time varying systems. Halkin also conjectures that other existence theorems in the theory of optimal control could be similarly strengthened.

It is doubtful, however, that it will ever be possible to state parallel, general existence results for the optimization problem stated in section 4.1, without relatively strong assumptions regarding the partial differential equations of the system, the control constraint set U and the functional I. Nevertheless, results in that direction have been recently

provided by Cesari (1971) for some problems of optimization with distributed and boundary controls.

When no existence theorem applies to the problem at hand one has to be content with presenting the best extremal control vector $\hat{\underset{\sim}{u}}(z,t)$ and relying on other knowledge about the problem to support the contention or at least the hope that it is the optimal control vector $\underset{\sim}{u}^{+}(z,t)$.

4.3.2. Extremal and Optimal Controls

The second task involves basically the solution of the state and costate equations (4-2) and (4-12) subject to their respective specified and transversality conditions (4-9), (4-13) and (4-14) using the maximum condition (4-15) or a weaker local maximum condition as is discussed in section 4.4.

The success of this endeavor depends to a large extent on whether or not it is possible to obtain a closed-form solution of the set of partial differential equations. If no closed-form solution is available, as often is the case, one must have recourse to a semi-analytical study of the problem, or, when even this is not possible, to a numerical method for solving the mixed end-point boundary problem.

Optimization problems for which the set of extremal control vectors $\hat{U}(z,t)$ is finite for each and every point $(z,t) \in \tau$ are commonly termed "normal" problems since the optimal control vector $\underset{\sim}{u}^{+}(z,t)$ if it exists can always be extracted, at least conceptually, out of such set.

Obviously, if the set $\hat{U}(z,t)$ consists of a unique extremal control vector $\hat{\underset{\sim}{u}}(z,t) \in U$ for each and every point $(z,t) \in \tau$ and if an optimal control vector $\underset{\sim}{u}^{+}(z,t)$ is known to exist in the whole of τ, then,

$$\underset{\sim}{u}^{+}(z,t) = \hat{\underset{\sim}{u}}(z,t) \qquad \text{all } z,t \in \tau \qquad (4\text{-}18)$$

defines an optimal control vector $\underset{\sim}{u}^+(z,t)$ uniquely determined in the whole of τ. If the set $\hat{U}(z,t)$ consists of one or many extremal control vectors $\hat{\underset{\sim}{u}}(z,t)$ at each and every point $(z,t) \in \tau$, one must upon identifying each extremal control vector $\hat{\underset{\sim}{u}}(z,t)$ in τ, compute the functional (4-10) associated with each of them and compare the corresponding numerical values in order to discriminate and determine the best extremal control vector $\hat{\underset{\sim}{u}}(z,t) \in \hat{U}(z,t)$. Thus when an optimal control vector $\underset{\sim}{u}^+(z,t)$ is known to exist,

$$\underset{\sim}{u}^+(z,t) = \{\hat{\underset{\sim}{u}}(z,t) \in \hat{U}(z,t) \;\Big|\; \text{minimum } I[\hat{\underset{\sim}{u}}(z,t)]\} \tag{4-19}$$

When more than one control vector $\hat{\underset{\sim}{u}}(z,t) \in \hat{U}(z,t)$ gives the same numerical result for the functional I, then the optimal control $\underset{\sim}{u}^+(z,t)$, existing, is not unique in τ.

4.4. A Local Maximum Condition

An extremal control vector $\hat{\underset{\sim}{u}}(z,t) \in U$ is characterized at any $(z,t) \in \tau$ by the fact that the maximum condition,

$$\Delta H = \left\{H[\hat{\underset{\sim}{u}} + \Delta\underset{\sim}{u}] - H[\hat{\underset{\sim}{u}}]\right\} \leq 0 \tag{4-20}$$

for <u>all finite admissible</u> control variations $\Delta\underset{\sim}{u}$,

$$(\hat{\underset{\sim}{u}} + \Delta\underset{\sim}{u}) \in U \tag{4-21}$$

Although this condition is conceptually useful in expressing the quality of extremal control vectors $\hat{\underset{\sim}{u}}(z,t) \in U$, which are candidates for optimality, it may prove difficult, in general, to use it directly as a global

procedure for finding the extremal control vectors $\hat{\underset{\sim}{u}}(z,t) \in U$ at points $(z,t) \in \tau$.

However, condition (4-20) validated for <u>all changes</u> $\Delta\underset{\sim}{u}$ consistent with condition (4-21) may be relaxed by using it to express the maximum condition that an extremal control vector $\hat{\underset{\sim}{u}}(z,t) \in U$ must obey <u>locally</u> with respect to other control vectors $\underset{\sim}{u}(z,t) \in U$ within some small neighbourhood of $\hat{\underset{\sim}{u}}(z,t)$, that is,

$$\Delta H = \left\{ H[\hat{\underset{\sim}{u}} + \delta\underset{\sim}{u}] - H[\hat{\underset{\sim}{u}}] \right\} \leq 0 \tag{4-22}$$

for <u>all infinitesimal admissible</u> control variations $\delta\underset{\sim}{u}$,

$$(\hat{\underset{\sim}{u}} + \delta\underset{\sim}{u}) \in U \tag{4-23}$$

Thus to find the absolute maximum of the function H over all $\underset{\sim}{u}(z,t) \in U$, one need only compare the value of the function H corresponding to each of the comparatively few local maxima and pick the control vector(s) $\hat{\underset{\sim}{u}}(z,t) \in U$ corresponding to the largest value of the function H.

The above scheme can be put to effect by constructing a test for local maxima. The key is the fact that only infinitesimal changes $\delta\underset{\sim}{u}$ need be considered.

Since at any point $(z,t) \in \tau$ the scalar function H is at least twice continuously differentiable with respect to the admissible control vectors $\underset{\sim}{u}(z,t) \in U$, a Taylor's series expansion of expression (4-22) would give,

$$\Delta H = \sum_{i=1}^{r} \frac{\partial H}{\partial u_i}\bigg|_{\hat{u}_i} \cdot \delta u_i + \frac{1}{2} \sum_{i=1}^{r} \sum_{j=1}^{r} \frac{\partial}{\partial u_i} \cdot \frac{\partial H}{\partial u_j}\bigg|_{\hat{u}_i,\hat{u}_j} \cdot \delta u_i \cdot \delta u_j + \Theta\left[(\underset{\sim}{\delta u})^3\right] \tag{4-24}$$

4.4.1. Interior Points

Now for an extremal control vector $\underset{\sim}{\hat{u}}(z,t) \in (\underset{\sim}{u}_*, \underset{\sim}{u}^*)$, small control variations $\underset{\sim}{\delta u}$ satisfying condition (4-23) may be arbitrarily either positive or negative. As $\underset{\sim}{\delta u} \to 0$, first-order variations of H will predominate and a necessary condition for a local maximum is that,

$$\frac{\partial H}{\partial \underset{\sim}{u}}\bigg|_{\underset{\sim}{\hat{u}}} = 0 \tag{4-25}$$

When this condition is met, equation (4-24) reduces to,

$$\Delta H = \frac{1}{2} \sum_{i=1}^{r} \sum_{j=1}^{r} \frac{\partial}{\partial u_i} \cdot \frac{\partial H}{\partial u_j}\bigg|_{\hat{u}_i,\hat{u}_j} \cdot \delta u_i \cdot \delta u_j + \Theta\left[(\underset{\sim}{\delta u})^3\right] \tag{4-26}$$

Letting $\underset{\sim}{\delta u} \to 0$, since $\Theta[(\underset{\sim}{\delta u})^3]$ goes faster to zero than $\Theta[(\underset{\sim}{\delta u})^2]$ and provided second-order variations of H are not all zero, these will predominate and an additional condition is that,

$$\sum_{i=1}^{r} \sum_{j=1}^{r} \frac{\partial}{\partial u_i} \cdot \frac{\partial H}{\partial u_j}\bigg|_{\hat{u}_i,\hat{u}_j} \cdot \delta u_i \cdot \delta u_j \leq 0 \tag{4-27}$$

in order that a local maximum condition (4-22) be met.

4.4.2. Boundary Points

When an extremal control vector $\hat{\underset{\sim}{u}}(z,t) = \partial U$, where ∂U represents the boundary of the set of admissible control vectors U, small control variations $\underset{\sim}{\delta u}$ are no longer arbitrary in regard to polarity, and,

$$\delta u_i > 0 \qquad \text{for} \quad \hat{u}_i = u_{i*} \tag{4-28}$$

and

$$\delta u_i < 0 \qquad \text{for} \quad \hat{u}_i = u_i^* \tag{4-29}$$

must satisfy condition (4-23).

Provided all first-order variations of the function H with respect to an extremal control $\hat{u}_i(z,t)$, i=1,...,r are not zero, they will predominate in equation (4-24) letting $\underset{\sim}{\delta u} \to 0$, and,

$$\sum_{i=1}^{r} \left. \frac{\partial H}{\partial u_i} \right|_{\hat{u}_i} \cdot \delta u_i \leq 0 \tag{4-30}$$

becomes a necessary condition for condition (4-22) to be satisfied there.

4.5. Linearity in Control

An important special case of the optimal control problem defined previously is obtained when one or more components $u_k(z,t)$ of the control vector $\underset{\sim}{u}(z,t) \in U$ enter the system equations (4-2) and function G_i of equation (4-10) in a linear manner. That is, when the i^{th} component of the vector $\underset{\sim}{f}$ for

the i^{th} scalar equation (4-2) is written as,

$$f_i[z,t,\underset{\sim}{\phi},\underset{\sim}{u}] = g_i[z,t,\underset{\sim}{\phi},\underset{\sim}{u}^n] + \sum_{k=1}^{m} u_k \cdot h_{ik}[z,t,\underset{\sim}{\phi},\underset{\sim}{u}^n] \qquad i=1,\ldots,n \tag{4-31}$$

and the function G_1 expressed as,

$$G_1[\underset{\sim}{\phi},\underset{\sim}{u}] = G_1'[\underset{\sim}{\phi},\underset{\sim}{u}^n] + \sum_{k=1}^{m} u_k \cdot H_k'[\underset{\sim}{\phi},\underset{\sim}{u}^n] \tag{4-32}$$

with

$$\underset{\sim}{u}^{\ell} = [u_1(z,t),\ldots, u_m(z,t)] \tag{4-33}$$

$$\underset{\sim}{u}^{n} = [u_{m+1}(z,t),\ldots, u_r(z,t)] \tag{4-34}$$

and

$$\underset{\sim}{u} = [\underset{\sim}{u}^{\ell},\underset{\sim}{u}^{n}] \tag{4-35}$$

The function H may then be written,

$$H = \Lambda[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^n] + \sum_{k=1}^{n} u_k \cdot \Gamma_k[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^n] \tag{4-36}$$

and is linear in the control components $u_k(z,t) \in \underset{\sim}{u}^{\ell}$, with

$$\Lambda[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^n] = G_1'[\underset{\sim}{\phi},\underset{\sim}{u}^n] + \sum_{i=1}^{n} \psi_i(z,t) \cdot g_i[z,t,\underset{\sim}{\phi},\underset{\sim}{u}^n] \tag{4-37}$$

and

$$\Gamma_k[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^n] = H_k'[\underset{\sim}{\phi},\underset{\sim}{u}^n] + \sum_{i=1}^{n} \psi_i(z,t) \cdot h_{ik}[z,t,\underset{\sim}{\phi},\underset{\sim}{u}^n] \tag{4-38}$$

The functions $\Gamma_k[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^n]$ are called the switching functions for the component $u_k(z,t) \in \underset{\sim}{u}^\ell$ and represent the gradient of the function H with respect to $u_k(z,t)$ all other variables remaining constant.

Thus if $\hat{\underset{\sim}{u}}(z,t)$ is an optimal control vector and if $\hat{\underset{\sim}{\psi}}(z,t)$ and $\hat{\underset{\sim}{\phi}}(z,t)$ represent the corresponding state and adjoint variable extremal trajectories, then in view of the function H defined in (4-36) and the maximum condition (4-15), each component $\hat{u}_k(z,t) \in \underset{\sim}{u}^\ell$ is formally given by,

$$\hat{u}_k(z,t) = \begin{cases} u_k^* & \text{for } \Gamma_k[z,t,\hat{\underset{\sim}{\phi}},\hat{\underset{\sim}{\psi}},\hat{\underset{\sim}{u}}^n] > 0 \\ \\ u_{k*} & \text{for } \Gamma_k[z,t,\hat{\underset{\sim}{\phi}},\hat{\underset{\sim}{\psi}},\hat{\underset{\sim}{u}}^n] < 0 \end{cases} \tag{4-39}$$

for k=1,...,m and where u_{k*} and u_k^* are respectively the lower and upper bounds on admissible values of $u_k(z,t) \in U$. Equation (4-39) may also be written in the alternate form:

$$\hat{u}_k(z,t) = \frac{1}{2}\{(u_k^*-u_{k*}) \cdot \text{sign}\,(\Gamma_k[z,t,\hat{\underset{\sim}{\phi}},\hat{\underset{\sim}{\psi}},\hat{\underset{\sim}{u}}^n]) + (u_k^*+u_{k*})\} \tag{4-40}$$

for k=1,...,m.

Extremal controls of the form given in equation (4-39) occur frequently in practice and are commonly referred to as "bang-bang" controls.

The switching function $\Gamma_k[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^n]$ is, in principle, determined as an explicit function of time and space by substituting equation (4-40) into the function H defined by equation (4-36) and solving the state and costate equations (4-2) and (4-12) subject to their respective initial and boundary values (4-8), (4-13), (4-9) and (4-14) and knowing the control vector $\underset{\sim}{u}^n$.

This procedure when realized, should yield a well-defined piecewise continuous control $\hat{u}_k(z,t)$ as long as their switching functions $\Gamma_k[z,t,\hat{\underset{\sim}{\phi}},\hat{\underset{\sim}{\psi}},\hat{\underset{\sim}{u}}^n]$ have only isolated zeros in τ.

4.5.1. Singular Problems

While it is possible in some particular problems [Leitmann (1959)] to rule out the possibilities of a switching function (4-38) vanishing on a non-empty subset $\Delta\tau \subseteq \tau$, this cannot be done in general.

In fact, there may exist an extremal control vectory $\hat{\underset{\sim}{u}}(z,t)$ distributed in the whole of τ such that the corresponding state $\hat{\underset{\sim}{\phi}}(z,t)$ and costate $\hat{\underset{\sim}{\psi}}(z,t)$ extremal trajectories render one or more than one of the k^{th} component of the switching function vector $\underset{\sim}{\Gamma}$ to vanish on a non-empty subset $\Delta\tau$.

Therefore, in the process of selecting the optimal control trajectory $\overset{+}{\underset{\sim}{u}}(z,t)$, existing for all $z,t \in \tau$, among the candidate extremal controls $\hat{\underset{\sim}{u}}(z,t) \in U$ one must, to avoid overlooking qualified candidates, admit into competition all those control candidates which may possibly be characterized by this condition.

It is characteristic of such an optimal control problem that when a switching function Γ_k becomes identically zero over a non-empty domain $\Delta\tau \subseteq \tau$, the function H defined in (4-36) no longer depends explicitly on the control variable $u_k(z,t)$ there, and the usual procedure of selecting $\hat{u}_k(z,t)$ so as to maximize the function H breaks down.

That is, the maximum condition (4-15) is trivially satisfied there and fails to provide an adequate test for the optimality of the control trajectory $u_k(z,t)$ in $\Delta\tau$ and correspondingly equations (4-39) and (4-40) fail to yield a well-defined control $\hat{u}_k(z,t)$ in $\Delta\tau$. Problems of that nature are referred to as singular.

Along extremal trajectories of the state and costate variables $\underset{\sim}{\phi}(z,t)$ and $\underset{\sim}{\psi}(z,t)$ everywhere defined in τ, the behaviour of each switching function Γ_k, k=1,...,m, may be classified into two distinct categories:

i - the condition $\Gamma_k = 0$ is satisfied along such extremal trajectories for all (z,t) belonging to non-empty open subsets $\delta\tau_1 \in \Delta\tau_1$ where $\Delta\tau_1 \subseteq \tau$ represents the union of these subsets. For all points (z,t) contained in each and every subset $\delta\tau_1 \in \Delta\tau_1$ the extremal control $\hat{u}_k(z,t)$ cannot be defined by equation (4-39). Such controls are referred to as singular.

ii - the zeros of the particular switching function Γ_k along such extremal trajectories are isolated in the whole of the subset $\Delta\tau_2$, where

$$\Delta\tau_2 = \tau \backslash \Delta\tau_1 \tag{4-41}$$

and the extremal control $\hat{u}_k(z,t)$ along such trajectories is well defined there according to equation (4-39).

Therefore, extremal control policies $\hat{u}_k(z,t)$ in τ, k=1,...,m, may consist only of "bang-bang" control policies, singular control policies or composite "bang-bang" and singular control sub-policies depending whether the set of points $(z,t) \in \tau$ where the controls are defined belongs entirely to the subset $\Delta\tau_2$, $\Delta\tau_1$ or partly in both.

Singular control candidates are characterized by the condition that in the interior of non-empty open subsets $\delta\tau_1$, the switching function Γ_k, $k \in [1,m]$, is identically zero and that all of its partial derivatives with respect to z and t, when they exist, are also zero:

$$\Gamma_k \equiv \frac{\partial^q \Gamma_k}{\partial t^q} = 0 \qquad q=1,2,\ldots;\ k \in [1,\ldots,m] \tag{4-42}$$

with

$$\Gamma_k \equiv \frac{\partial^{q'} \Gamma_k}{\partial z^{q'}} = 0 \qquad q'=1,2,\ldots;\ k \in [1,\ldots,m] \tag{4-43}$$

It should be stressed, however, that the existence of singular control candidates does not necessarily imply the existence of singular control sub-arcs to the optimal control problem [Johnson (1965)].

The possible appearance of singular control sub-arcs in the optimal control problem is accompanied by considerable analytical difficulty.

A major problem is that at present there is still no generally applicable analytical method for the distributed parameter optimal control problem by which one can ascertain a priori whether a singular control candidate in $\Delta\ \tau_1$ actually represents any part of an extremal control trajectory in τ.

Also, since in general the points of transition from singular control sub-arcs to "bang-bang" control sub-arcs (and vice versa) must be determined from consideration of the mixed end-point boundary problem, no general analytical method is available for determining these control sub-arcs and the manner in which they form segments of the entire extremal control policy for both the lumped and distributed parameter control problems.

Singularities have been known to appear in classical lumped parameter variational problems and the corresponding singular problem arising from the use of maximum principle of Pontryagin et al. (1962) has also been recognized [Johnson and Gibson (1963)].

Research interest in this area has been mainly directed towards three major aspects of the problem, namely:

i - the derivation of necessary and sufficient optimality conditions that must be obeyed on a singular sub-arc.

ii - the establishment of conditions that must be necessarily met at the junction points where non-singular control sub-arcs join singular control sub-arcs (and vice versa).

iii - developing transformation techniques by which a singular problem might be transformed to a non-singular one.

As a result of activities concerned with the first item, a necessary, but not sufficient, condition for a singular trajectory to be optimal with respect to an arbitrary piecewise continuous perturbation in the singular control sub-arc has been discovered by Kelley (1964). This condition was generalized subsequently by Robbins (1966), Tait (1965), Kelley et al. (1967) and Goh (1966) and is now commonly known as the generalized Legendre-Clebsch condition, or:

$$(-1)^q \frac{\partial}{\partial u_k} \cdot \left[\frac{d^{2q}}{dt^{2q}} \cdot \left(\frac{\partial H}{\partial u_k}\right)\right] \leq 0 \qquad q=1,2,\ldots;\ k \in [1,2,\ldots,m] \qquad (4\text{-}44)$$

This result expresses the fact that for a specially chosen class of piecewise continuous perturbations in the singular control sub-arc, the second variation of the cost functional along a singular trajectory is strictly positive if and only if the inequality sign is satisfied.

Using a different special control variation in the singular control sub-arc, Gabasov (1968, 1969) later obtained an additional necessary condition to the Legendre-Clebsch condition for the case of unconstrained terminal state.

This condition was also found, independently, by Jacobson (1969) whose treatment also included constraints on the terminal state. It has been recently shown, however, that both this additional necessary condition and the Legendre-Clebsch condition are still insufficient for optimality [Jacobson (1970_b)].

Sufficient conditions for non-negativity of the second variation in singular and non-singular problems have been presented lately by Jacobson (1970_a). These conditions in the form of equalities and differential inequalities are sufficient for a weak relative minimum of the cost functional. It is also shown that these conditions are applicable to totally singular, partially singular and non-singular control functions.

A rather thorough analysis has been carried out also for the linear, constant coefficient system with the performance index quadratic in the state [Kliger (1964), Wonham (1964)]. McDanell and Powers (1970) recently obtained a new Jacobi-type necessary and sufficient condition for these systems but for which the control trajectory is totally singular in the whole domain of the problem.

All of these results pertain to lumped parameter optimal control systems, and, with the exception of a worthy but unsuccessful effort by Seinfeld (1967) to derive a corresponding Legendre-Clebsch condition for the distributed parameter optimal control problem, no other result pertaining to this latter field has appeared, to the author's knowledge, in the open literature.

Activities relating to the second item have resulted in worthwhile observations by Kelley, Kopp and Moyer (1967) concerning the possibility of jump discontinuities in the control at the junction points of non-singular with singular (and vice versa) control sub-arcs.

Independent results and stronger necessary conditions have been given by Johnson (1965) using geometrical conditions which must be satisfied for the singular trajectory to be reachable by a non-singular trajectory corresponding to both limits of a non-singular control sub-arc.

The latest contribution in that direction has been made by Seinfeld (1967) who extended Johnson's result to include consideration of a class of distributed parameter systems.

Investigations pertaining to transformation techniques related to lumped parameter systems have been done by Kelley (1965) and Goh (1966) by which a singular problem may be transformed to a non-singular one, thereby allowing application of the classical necessary optimality conditions. However, the transformations required are often cumbersome and do not guarantee that a non-singular problem will result from its use.

The most important question of synthesis of optimal controls in general non-linear problems in which singularities may exist, except for recent computational algorithms by Jacobson and Lele (1970) for the lumped parameter systems and some computational effort by Seinfeld (1967) to distributed parameter systems, has largely been avoided.

CHAPTER 5

ANALYSIS OF THE OPTIMALITY PROBLEM

The precise statement of the optimization problem for the quasi-steady state reaction-deactivation process is given in section 3.3.2. and represents a particular and simplified form of the general optimization formulation given in section 4.1.

5.1. A Maximum Principle Formulation for the Quasi-Steady State Problem

Treated in the format and nomenclature of the maximum principle enunciated by Sirazetdinov and Degtyarev (1967) and retaining for clarity the definition and nomenclature of the catalytic reaction-deactivation system given in Chapter 3, the equivalence resulting between the symbols is given in Table 5-1 for the general unsteady state process.

With that set of definitions, the minimization of the functional I defined by equation (4-10) corresponds to the maximization of the cost functional J defined by equation (3-41).

The system equations (3-30) with (3-32) describing the unsteady state process and (3-31) with (3-32) for the quasi-steady state process are totally hyperbolic in the whole domain considered (see Appendix A) and the maximum principle formulation thus becomes for the unsteady state process,

$$H[X,\psi,\lambda,\mu,k] = \lambda.F[X].K[k].\psi - \mu.k.g[\psi] \qquad (5\text{-}1)$$

with the costate variables defined as,

DESCRIPTION	Sirazetdinov Degtyarev (1967)	This Work
Domain	$\tau = Z^o \times T^o$	$\tau = Z^o \times T^o$
	$T^o = [t_o, t_f]$	$T^o = [0,1]$
	$Z^o = [z_o, z_f]$	$Z^o = [0,1]$
Independent Variables	$z \in Z^o$	$z \in Z^o$
	$t \in T^o$	$t \in T^o$
State Variables [n = 2]	$\Phi_1(z,t)$	$X(z,t)$
	$\Phi_2(z,t)$	$\psi(z,t)$
Costate Variables [n = 2]	$\psi_1(z,t)$	$\lambda(z,t)$
	$\psi_2(z,t)$	$\mu(z,t)$
Control Variable [r = 1]	$\mu_1(z,t)$	$k(z,t)$
System Coefficients [n = 2]	$a_{11}(z,t)$	(t_f/t_Θ)
	$a_{12}(z,t)$	o.
	$a_{21}(z,t)$	o.
	$a_{22}(z,t)$	o.
Functions [n = 2]	$f_1[z,t,\Phi,\mu]$	$\psi.K[k].F[X]$
	$f_2[z,t,\Phi,\mu]$	$- k.g[\psi]$
Functional Components	$G_1[\Phi,\mu]$	o.
	$G_2'[\Phi(z_o,t)]$	$X(o,t)$
	$G_2''[\Phi(z_f,t)]$	$- X(1,t)$
	$G_3[\Phi(z,t_f)]$	o.

Table 5-1 Symbol Equivalence

$$\frac{\partial \lambda}{\partial t} + (t_f/t_\Theta) \cdot \frac{\partial \lambda}{\partial z} = - \frac{\partial H}{\partial X} = - \lambda . F'[X] . \psi . K \qquad (5\text{-}2)$$

and

$$\frac{\partial \mu}{\partial t} = - \frac{\partial H}{\partial \psi} = \lambda . F[X] . K - \mu . k . g'[\psi] \qquad (5\text{-}3)$$

with, for the monotonic decreasing function $F[X]$ of X, or constant $F[X]$,

$$F'[X] = \frac{d\ F[X]}{dx} \leqslant 0 \qquad (5\text{-}4)$$

and, for the monotonic increasing function $g[\psi]$ of ψ, or constant $g[\psi]$,

$$g'[\psi] = \frac{d\ g[\psi]}{d\ \psi} \geqslant 0 \qquad (5\text{-}5)$$

The associated terminal and boundary conditions corresponding to equations (4-13) and (4-14) are,

$$\lambda(z,1) = 0 \qquad \text{all } z \in [o,1] \qquad (5\text{-}6)$$

$$\lambda(1,t) = (t_\Theta/t_f) \qquad \text{all } t \in [o,1] \qquad (5\text{-}7)$$

$$\mu(z,1) = 0 \qquad \text{all } z \in [o,1] \qquad (5\text{-}8)$$

For conditions pertaining to the quasi-steady state process, it is shown in Appendix C that the corresponding maximum principle becomes:

$$H[X,\psi,\lambda,\mu,k] = \lambda . F[X] . \psi . K - \mu k . g[\psi] \qquad (5\text{-}9)$$

with the costate variables now defined as,

$$(t_f/t_\Theta) \cdot \frac{\partial \lambda}{\partial z} = - \frac{\partial H}{\partial X} = - \lambda.F'[X].\psi.K \qquad (5\text{-}10)$$

and

$$\frac{\partial \mu}{\partial t} = - \frac{\partial H}{\partial \psi} = - \{\lambda.F[X].K - \mu.k.g'[\psi]\} \qquad (5\text{-}11)$$

The associated terminal and boundary conditions are given by (5-8) and (5-7).

5.2. Basic Characteristics of Extremal Control Policies

The nature of extremal control policies pertaining to the quasi-steady state system may be identified using the global maximum condition (4-16) for controls,

$$k_* \leqslant k^+(z,t) \leqslant k^* \qquad (5\text{-}12)$$

and where,

$$\Delta H = \lambda.F[X].\psi.\Delta K - \mu.g[\psi].\Delta k \qquad (5\text{-}13)$$

with Δk such that,

$$[k^+(z,t) + \Delta k] \in [k_*, k^*] \qquad (5\text{-}14)$$

However, if $k^+(z,t)$ is an optimal control, then one of the following conditions, given by equations (4-25), (4-27) and (4-30), is necessary at any point $(z,t) \in \tau$:

$$i \quad - \quad \left.\frac{\partial H}{\partial k}\right|_{k^+} = 0 \qquad \text{if } k_* < k^+(z,t) < k^* \qquad (5\text{-}15)$$

with

$$\left.\frac{\partial^2 H}{\partial k^2}\right|_{k^+} \leq 0 \qquad \text{for } k_* < k^+(z,t) < k^* \qquad (5\text{-}16$$

$$ii \quad - \quad \left.\frac{\partial H}{\partial k}\right|_{k^+} \geq 0 \qquad \text{if } k^+(z,t) = k^* \qquad (5\text{-}17)$$

$$iii \quad - \quad \left.\frac{\partial H}{\partial k}\right|_{k^+} \leq 0 \qquad \text{if } k^+(z,t) = k_* \qquad (5\text{-}18)$$

where

$$\frac{\partial H}{\partial k} = \frac{p.\lambda.F[X].\psi.K}{k} - \mu.g[\psi] \qquad (5\text{-}19)$$

with

$$\frac{\partial^2 H}{\partial k^2} = \frac{p.(p-1).\lambda.F[X].\psi.K}{k^2} \qquad (5\text{-}20)$$

A control policy which fulfills these local and necessary conditions is not guaranteed to be optimal and has been discussed in sections 4.3 and 4.4.

Control policies characterized by conditions (5-15), (5-17) and (5-18) respectively are referred to in this study as a stationary policy S, a policy C* and a policy C_*. Therefore, an extremal control policy $\hat{k}(z,t)$ at any station $z \in [o,1]$ may consist, in time, of one or more control sub-policies drawn from types S, C^* or C_*.

The parameter p, entering directly equations (5-19) and (5-20) plays a decisive role in the admissibility of a control sub-policy to an extremal control policy. Consideration of limits for the value of p clearly illustrates this fact.

For $p = 0$, the reaction rate is independent of temperature and as low a temperature as possible should be chosen in order to retain the highest possible catalyst activity level in the reactor. For $p = \infty$, the deactivation rate is virtually independent of the temperature and as high a temperature as possible should be chosen in order to achieve the highest possible conversion level.

Several characteristics of extremal control policies have been identified for intermediate ranges of the value of the parameter p and are discussed for the following cases:

i - $0 < p < 1$

ii - $1 < p < \infty$

iii - $p = 1$

Results are given with proofs and are stated in the form of properties and sub-properties of the optimization problem. Termination of a proof is indicated by using the geometrical symbol ★.

Trivial situations where the initial catalyst activity distribution $\psi_0(z)$, $z \in [0,1]$ is identically zero or that the inlet conversion $X_0(t)$, $t \in [0,1]$ is the maximum attainable conversion, X_1^*, are ignored.

A common characteristic of an extremal control policy holding for positive values of the parameter p is summarized by the following two properties. It is established first, with the stated assumption, that at

$t = 1$, all extremal control policies must end at $k(z',1) = k^*$ everywhere in the reactor.

Property 1:

> If for all $z \in [o,1]$, $\psi(z,1) \cdot F[X(1,1)] > 0$, then
> $\hat{k}(z,1) = k^*$ all $z \in [o,1]$

Proof:

At $t = 1$, by (5-11), $\mu(z,1) = 0.$ for all $z \in [o,1]$ and (5-19) reduces to,

$$\left.\frac{\partial H}{\partial k}\right|_{t=1} = \frac{p.\lambda(z,1).\psi(z,1).F[X(z,1)].K(z,1)}{k(z,1)} \tag{5-21}$$

or using equation (D-18),

$$\left.\frac{\partial H}{\partial k}\right|_{t=1} = \frac{p.\psi(z,1).F_1(1).K(z,1)}{k(z,1)} \tag{5-22}$$

Finally for $\psi(z,1).F[X(1,1)] > 0$ and all $z \in [o,1]$, this expression contains only positive terms for all admissible control values $k_* \leqslant k(z,1) \leqslant k^*$ and the function H,

$$H\Big|_{t=1} = \psi(z,1).F_1(1) \cdot K(z,1) \tag{5-23}$$

with $K(z,1) \alpha k(z,1)$ can be increased by any admissible increase of the control

value $k(z,1)$. Thus

$$\hat{k}(z,1) = k^* \qquad \text{all} \quad z \in [o,1] \tag{5-24}$$

★

It is demonstrated in the following, with the stated assumption, that all extremal control policies consist at least of a control sub-policy C* in time $1 - \delta t_o < t \leqslant 1$ with $\delta t_o > 0$ everywhere in the reactor.

Property 2:

> If for all $z \in [o,1]$, $\psi(z,1).F[X(1,1)] > 0$, then for $\delta t_o > 0$,
> $k(z,t) = k^*$ all $z \in [o,1]$, $1 - \delta t_o < t \leqslant 1$

Proof:

The inlet conversion $X_o(t)$ having been assumed to be a piecewise continuous function of time, there exists a time interval δt such that $X_o(t)$ is continuous for $1 - \delta t < t \leqslant 1$. On such a time interval, consideration of (5-19) upon substitution of (D-18) gives,

$$\frac{\partial H}{\partial k} = \frac{p.F_1(t).K.\psi}{k} - \mu.g[\psi] \tag{5-25}$$

At $t = 1$, $\mu(z,1) = 0$. for all $z \in [o,1]$ and, with the stated assumption, the condition,

$$\left.\frac{\partial H}{\partial k}\right|_{t=1} = \frac{p.F_1(1).K.\psi}{k} > 0 \tag{5-26}$$

is recovered.

Since the functions $\mu(z,t)$ and $\psi(z,t)$ are continuous in time (see Appendix D) and the function $\frac{\partial H}{\partial k}$ is a continuous function of its arguments, there must exist, corresponding to each $z \in [o,1]$, a finite time interval $\delta t \geq \delta t_o > 0$ such that,

$$\left.\frac{\partial H}{\partial k}\right|_t > 0 \qquad (1 - \delta t_o) < t \leq 1 \qquad (5\text{-}27)$$

for all admissible controls $k(z,t) \in [k_*, k^*]$. Thus the function H could be increased by any admissible increase in $k(z,t)$ unless $k(z,t) = k^*$ and so,

$$\hat{k}(z,t) = k^* \qquad \text{all } z \in [o,1],\ (1 - \delta t_o) < t \leq 1 \qquad (5\text{-}28)$$

★

5.3. $0 < p < 1$

The kinetic significance of the parameter $p \in (0,1)$ is that an increase of the operating temperature would increase the rate constant $k[T]$ for catalyst decay faster than the rate constant $K[T]$ for reaction. Although such control action would not appear desirable, a lowering of the operating temperature in order to retain a high catalyst activity level in the reactor would result in a decrease in the rate constant $K[T]$ for reaction.

This apparent conflict in the choice of a control policy seems to indicate that a "best" compromise between these two situations would exist such that at points $(z,t) \in \tau$ a control $k(z,t)$ could be adjusted in order to minimize the rate of decay and maximize the rate of reaction.

This indication, based on rather intuitive concepts, is established in the following property.

Property 3:

> When $\psi(z,t).F[X(1,t)] > 0$ for all $z,t \in \tau$, then a stationary control policy S is an admissible control sub-policy to an extremal control policy.

Proof:

Condition (5-16), upon substitution of (D-18), may be written,

$$\frac{\partial^2 H}{\partial k^2} = \frac{p.(p-1).\ F_1(t)\ .\ \psi(z,t).K(z,t)}{k^2} \qquad (5\text{-}29)$$

Given the assumption that $\psi(z,t).F[X(1,t)] > 0$ everywhere in τ, the second partial derivative (5-29) is strictly negative everywhere in τ for values of $0 < p < 1$ and constitutes a sufficient condition for the function H to be locally a maximum on a stationary control policy S.

By properties 1 and 2, with the given assumption, this admissible stationary control policy S to an extremal control policy cannot alone constitute, at each and every station $z \in [o,1]$, a pure extremal control policy for all time $t \in [o,1]$. This completes the proof.

★

The maximum of the function H, however, is not guaranteed to correspond to a unique extremal control and has been discussed in section 4.3. Yet, the possibility of having multiple extremal controls $\hat{k}(z,t)$ at any given

point $(z,t) \in \tau$ is shown here not to exist and is summarized in the following.

Property 4:

> At any given point $(z,t) \in \tau$ for which the condition $\psi(z,t) \cdot F[X(1,t)] > 0$ exists, an extremal control $\hat{k}(z,t)$ is uniquely determined there.

Proof:

For $0 < p < 1$, the second partial derivative (5-29) with the stated assumption, is strictly negative for all admissible control values $k(z,t) \in [k_*, k^*]$ and,

$$\frac{\partial^2 H}{\partial k^2} < 0 \tag{5-30}$$

Therefore $\frac{\partial H}{\partial k}$ is not constant with varying $k(z,t)$ but can change sign if and only if the function H has a maximum with respect to $k(z,t) \in [k_*, k^*]$. Since condition (5-30) implies that the function H is a strictly concave function of the control $k(z,t)$ at any given point $(z,t) \in \tau$, the maximum of the function H is unique and the corresponding control,

$$k_* \leq \hat{k}(z,t) \leq k^* \tag{5-31}$$

is unique at that point.

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A direct consequence of that property, with the stated assumption, is that equations (5-15), (5-16), (5-17) and (5-18) represent a set of global conditions that an extremal $\hat{k}(z,t)$ must satisfy necessarily at any given point $(z,t) \in \tau$ in order to be optimal.

Moreover, this set of conditions now represents necessary and sufficient conditions that a control $k(z,t) \in [k_*,k^*]$ must obey in order to be an extremal control $\hat{k}(z,t)$ uniquely determined at any given point $(z,t) \in \tau$.

Typical curves of the function H with respect to admissible controls $\hat{k} \in [k_*,k^*]$ are illustrated in figure 5-1.

The joining of a stationary control policy S with a policy C* or C_* and the possible occurrence of a discontinuous transfer between control policies are investigated below.

Property 5:

> When $X_0(t)$ is a continuous function of time for $t\in[t_1,t_2]$ and if $\psi(z,t).F[X(1,t)] > 0$ everywhere in τ then finite jumps in control occurring simultaneously at a time $t_s^- \in (t_1,t_2)$ over a finite length $\Delta z \subseteq Z^0$ of the reactor are not optimal.

Proof:

Because of the strict concavity of the function H with respect to all admissible controls (see property 4) a jump in control at a time $t_s^- \in (t_1,t_2)$, where

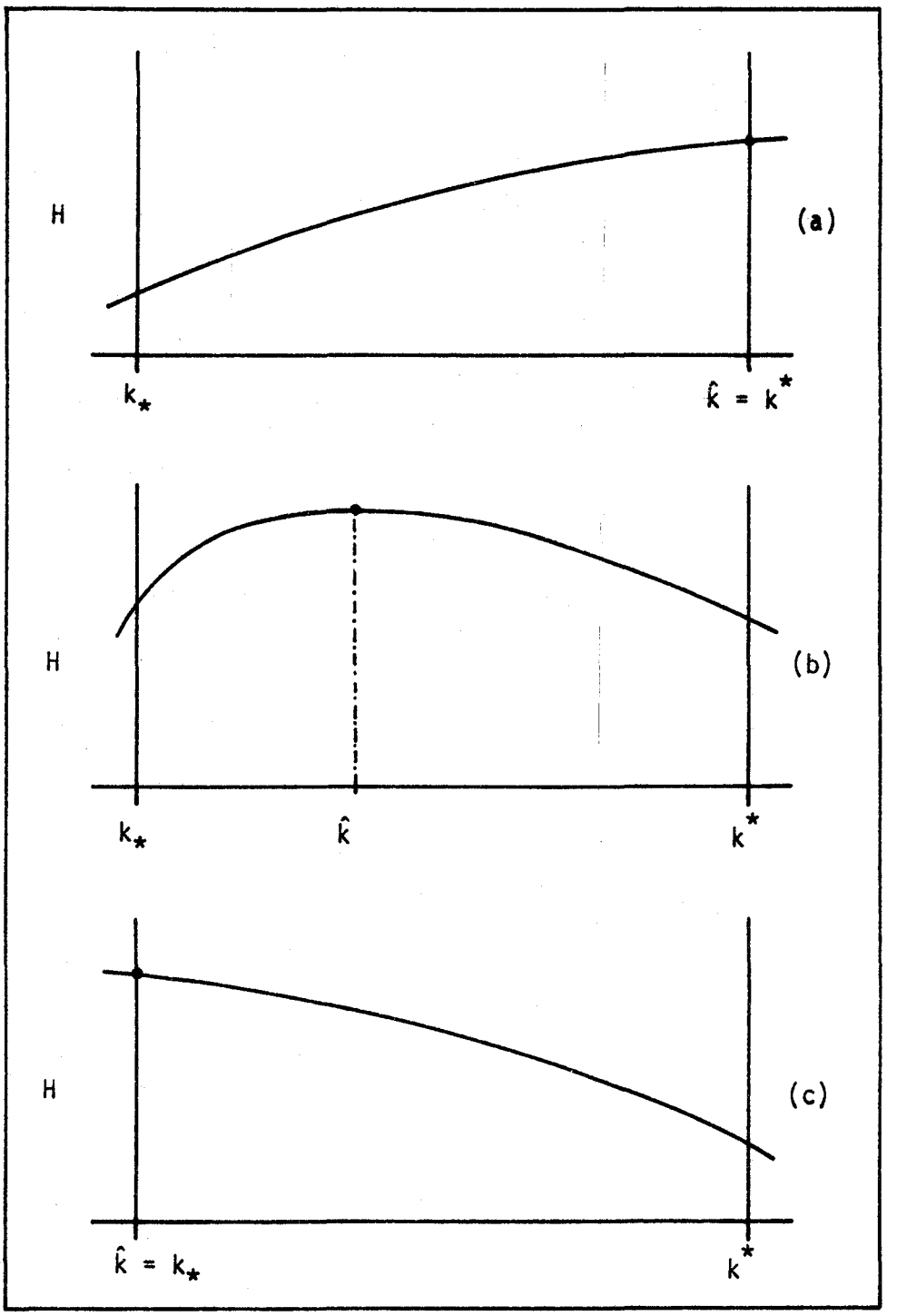

Figure 5-1 Typical Curves Of The Function H(z,t) Versus The Control $k_* \leq k(z,t) \leq k^*$ for $0 < p < 1$.

$$t_s^- = \text{limit}\left\{ t_s - \delta t \right\} \qquad (5\text{-}32)$$

$$\delta t > 0$$

$$\delta t \to 0$$

may exist iff the maxima of the function H at times t_s and t_s^- correspond to controls $\hat{k}(z,t_s)$ and $\hat{k}(z,t_s^-)$ whose values remain different by a finite quantity at the limit for $t_s^- \to t_s$. Necessary conditions for the optimality of finite jumps in control at any specific station $z \in [o,l]$ are,

$$\left.\frac{\partial H}{\partial k}\right|_{\hat{k}(z,t_s^-)} \geq \left.\frac{\partial H}{\partial k}\right|_{\hat{k}(z,t_s)} \quad \text{if} \quad \hat{k}(z,t_s^-) > \hat{k}(z,t_s) \qquad (5\text{-}33)$$

and

$$\left.\frac{\partial H}{\partial k}\right|_{\hat{k}(z,t_s^-)} \leq \left.\frac{\partial H}{\partial k}\right|_{\hat{k}(z,t_s)} \quad \text{if} \quad \hat{k}(z,t_s^-) < \hat{k}(z,t_s) \qquad (5\text{-}34)$$

where using (5-25) and recalling from (3-37) that $K = A.k^p$,

$$\left.\frac{\partial H}{\partial k}\right|_{\hat{k}(z,\varepsilon)} = \frac{p.A.\psi(z,\varepsilon).\ F_1(\varepsilon)}{[k(z,\varepsilon)]^{1-p}} - \mu(z,\varepsilon).g[\psi(z,\varepsilon)] \qquad (5\text{-}35)$$

with the positive constant A defined in (3-38). Since $\mu(z,t)$ and $\psi(z,t)$ are continuous functions of time, at the limit for $t_s^- \to t_s$,

$$\psi(z,t_s^-) = \psi(z,t_s) \qquad (5\text{-}36)$$

and

$$\mu(z,t_s^-) = \mu(z,t_s) \qquad (5\text{-}37)$$

equation (5-35) may be written for times t_s and $t_{\bar{s}}$ but at the limit for $t_{\bar{s}} \to t_s$,

$$\left.\frac{\partial H}{\partial k}\right|_{\hat{k}(z,t_s)} = \frac{p.A.\psi(z,t_s).\ F_1(t_s)}{[k(z,t_s)]^{1-p}} - \mu(z,t_s).g[\psi(z,t_s)] \qquad (5\text{-}38)$$

and

$$\left.\frac{\partial H}{\partial k}\right|_{\hat{k}(z,t_{\bar{s}})} = \frac{p.A.\psi(z,t_s).\ F_1(t_{\bar{s}})}{[k(z,t_{\bar{s}})]^{1-p}} - \mu(z,t_s).g[\psi(z,t_s)] \qquad (5\text{-}39)$$

The exit conversion $X(1,t)$, corresponding to a continuous inlet conversion $X_o(t)$ in time $t \in [t_1,t_2]$, is dependent upon the integral value of the controls along the whole length of the reactor in time and the effect of finite but admissible jumps in control occurring uniformly along a finite length of the reactor $\Delta z \subseteq Z^o$ at a time $t_{\bar{s}} \in (t_1,t_2)$ may result in only one of the following three possible cases:

$$X(1,t_{\bar{s}}) = X(1,t_s) \qquad (5\text{-}40)$$

$$X(1,t_{\bar{s}}) > X(1,t_s) \qquad (5\text{-}41)$$

$$X(1,t_{\bar{s}}) < X(1,t_s) \qquad (5\text{-}42)$$

It will be assumed in the following that finite but admissible jumps in control occur simultaneously at a time $t_{\bar{s}}$ at each and every station $\hat{z} \in \Delta z \subseteq Z^o$.

For the case of (5-40), since a jump in temperature in one direction only is not consistent with (5-40) it is necessary that along some finite segments of the reactor $\delta z \subset \Delta z$,

$$\hat{k}(\bar{z},t_{\bar{s}}) > \hat{k}(\bar{z},t_s) \qquad \text{all } \bar{z} \in \delta z \tag{5-43}$$

but from equations (5-38) and (5-39) at the limit for $t_{\bar{s}} \to t_s$,

$$\frac{\partial H}{\partial k}\bigg|_{\hat{k}(\bar{z},t_{\bar{s}})} < \frac{\partial H}{\partial k}\bigg|_{\hat{k}(\bar{z},t_s)} \qquad \text{all } \bar{z} \in \delta z \tag{5-44}$$

and result (5-44) contradicts optimality condition (5-33) corresponding to controls (5-43). The consideration of finite jumps in control leading to case (5-41) requires that along some finite segments of the reactor $\delta z \subseteq \Delta z$ the controls,

$$\hat{k}(\bar{z},t_{\bar{s}}) > \hat{k}(\bar{z},t_s) \qquad \text{all } \bar{z} \in \delta z \tag{5-45}$$

From equations (5-38) and (5-39) and recalling that $F[X]$ is a continuous monotonic decreasing (or constant) function of X, at the limit for $t_{\bar{s}} \to t_s$, result (5-44) is again obtained and optimality condition (5-33) corresponding to controls (5-45) is again contradicted.

Now when case (5-42) arises from the action of finite jumps in control over finite segments $\delta z \subseteq \Delta z$, that is,

$$\hat{k}(\bar{z},t_{\bar{s}}) < \hat{k}(\bar{z},t_s) \tag{5-46}$$

then from equations (5-38) and (5-39) at the limit for $t_{\bar{s}} \to t_s$,

$$\frac{\partial H}{\partial k}\bigg|_{\hat{k}(\bar{z},t_{\bar{s}})} > \frac{\partial H}{\partial k}\bigg|_{\hat{k}(\bar{z},t_s)} \qquad \text{all } \bar{z} \in \delta z \tag{5-47}$$

but this contradicts optimality condition (5-34) corresponding to controls (5-46).

Therefore, finite but admissible jumps in control occurring simultaneously in time along a finite length of the reactor $\Delta z \subseteq Z^o$ are not optimal.

✱

Since an optimal control policy may not contain any control discontinuity occurring simultaneously in time over a finite length of the reactor, that is a line of discontinuity parallel to the flow axis of the reactor, the conversion $X(z,t)$ resulting from such an optimal operation and corresponding to a continuous inlet conversion $X_o(t)$ in time is also a continuous function of time for all $z \in [o,1]$.

A direct consequence of that result is contained in the next stated sub-property.

Sub-Property 5a:

> When the inlet conversion $X_o(t)$ is a continuous function of time for $t \in [t_1,t_2]$ and if $\psi(z,t).F[X(1,t)] > 0$ everywhere in τ, then a finite jump in control occurring at a time $t_s \in (t_1,t_2)$ but at isolated stations $z_s \in [o,1]$ is also not optimal.

Proof:

Because of property 5, with the stated assumptions, the exit conversion $X(1,t)$ is a continuous function of time for all $t \in (t_1,t_2)$.

Therefore, corresponding to finite but admissible jumps in control at a time $t_{\bar{s}} \in (t_1,t_2)$ but at isolated stations $z_s \in [o,1]$, subject to the optimality conditions (5-33) and (5-34), case (5-40) needs only to be considered.

Since for finite but admissible jumps in control,

$$\hat{k}(z_s,t_{\bar{s}}) > \hat{k}(z_s,t_s) \qquad z_s \in [o,1] \tag{5-48}$$

or

$$\hat{k}(z_s,t_{\bar{s}}) < \hat{k}(z_s,t_s) \qquad z_s \in [o,1] \tag{5-49}$$

results (5-44) and (5-47) are obtained respectively for controls (5-48) and (5-49) and the optimality conditions (5-33) and (5-34) corresponding to controls (5-48) and (5-49) are in both cases contradicted at each and every isolated station $z_s \in [o,1]$.

Thus at each and every station of the reactor $z \in [o,1]$ no discontinuous control policy in time $t \in (t_1,t_2)$ may be optimal.

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Therefore, with the stated assumptions, all optimal control policies $k^+(z,t)$ at each and every station $z \in [o,1]$ are continuous functions of time. Also the function H and its gradient (5-19) are both continuous functions of time there. They have continuous first partial derivatives with respect to time for all $t \in T^o$ under consideration except possibly for a set of points on T^o, namely at times where the inlet conversion $X_o(t)$ and the control $k(z,t)$ may have a discontinuity of the first kind in their time derivatives. On an interval of time where the gradient (5-19) is

continuously zero,

$$\frac{\partial H}{\partial k}\Big|_{\hat{k}} = 0 \tag{5-50}$$

the partial derivative of the gradient with respect to time and existing continuously on that interval must also vanish and,

$$\frac{\partial}{\partial t} \cdot \frac{\partial H}{\partial k}\Big|_{\hat{k}} = 0 \tag{5-51}$$

where

$$\frac{\partial}{\partial t} \cdot \frac{\partial H}{\partial k} = \frac{\partial}{\partial t} \cdot \left\{ \frac{p.F_1.\psi.K + \mu.\phi}{k} \right\} \tag{5-52}$$

with,

$$\phi = - k.g[\psi] \tag{5-53}$$

and from (D-18)

$$F_1 = F_1(t) = \lambda(z,t).\ F[X(z,t)] \tag{5-54}$$

Because of conditions (5-50) and (5-51) equation (5-52) may be written,

$$\frac{\partial}{\partial t} \{p.F_1.\psi.K + \mu.\phi\} = 0 \tag{5-55}$$

or,

$$p.\psi.K.\ \frac{d\ F_1}{dt} + p.F_1.\ \frac{\partial \psi K}{\partial t} + \mu.\frac{\partial \phi}{\partial t} + \phi.\ \frac{\partial \mu}{\partial t} = 0 \tag{5-56}$$

Since

$$\frac{\partial \phi}{\partial t} = \frac{\partial \phi}{\partial \psi} \cdot \frac{\partial \psi}{\partial t} + \frac{\partial \phi}{\partial k} \cdot \frac{\partial k}{\partial t} \tag{5-57}$$

and recalling equations (3-32) and (5-11) equation (5-56) becomes with (5-53) and (5-54),

$$p.\psi.K. \frac{d F_1}{dt} + p.F_1. \frac{\partial \psi K}{\partial t} + \frac{\mu.\phi}{k} \cdot \frac{\partial k}{\partial t} - K.F_1.\phi = 0 \tag{5-58}$$

Also, from (5-19), (5-50) and (5-54),

$$\mu.\phi = - p.\psi.K.F_1 \tag{5-59}$$

and recalling that,

$$\frac{\partial k}{\partial t} = \frac{\partial k}{\partial K} \cdot \frac{\partial K}{\partial t} = \frac{k}{pK} \cdot \frac{\partial K}{\partial t} \tag{5-60}$$

relation (5-58) then becomes with (5-53) and (3-32),

$$p.\psi.K. \frac{d F_1}{dt} + p.F_1. \frac{\partial \psi K}{\partial t} - \psi.F_1. \frac{\partial K}{\partial t} - K.F_1. \frac{\partial \psi}{\partial t} = 0 \tag{5-61}$$

or grouping,

$$\frac{(1-p)}{p} \cdot \frac{\partial \ln \psi K}{\partial t} = \frac{d \ln F_1}{dt} \tag{5-62}$$

Integrating, at constant z, from a reference time t^o to a time t,

$$\psi.K = \psi(z,t).K(z,t) = \frac{\psi^o(z).K^o(z)}{(F_1^o)^\alpha} \cdot F_1^\alpha \tag{5-63}$$

where

$$\alpha = p/(1-p) \tag{5-64}$$

$$\psi^{o}(z) = \psi(z,t^{o}) \tag{5-65}$$

$$K^{o}(z) = K(z,t^{o}) \tag{5-66}$$

$$F_1^{\,o} = F_1(t^{o}) \tag{5-67}$$

The product ψK is called the local effective rate constant for reaction. From a knowledge of:

i - the desired or given exit conversion profile $X(1,t)$ in time, and,

ii - the effective rate constant at some specific reference time t^{o},

equation (5-63) permits the construction of a stationary control $\hat{k}(z,t)$ in time t at each and every station z for which condition (5-50) holds.

A characteristic of the effective rate constant for reaction, first noted by Crowe (1970), is that it is expressible as a product of separate functions, each depending respectively on only one independent variable z or t.

Now when the entire reactor is on a constrained control policy C^{*} and/or C_{*} for a time interval $\Delta t \subseteq T^{o}$, the exit conversion $X(1,t)$ corresponding to a non-varying inlet conversion $X_{o}(t)$ in time, is clearly a continuous and monotonic decreasing function of time since the controls $\hat{k}(z,t)$ are non-varying in time $t \in \Delta t$ and the relative catalyst activity level $\psi(z,t)$ is a continuous and monotonic decreasing function of time.

When at any one time t, parts of the bed are on a stationary control policy S and other parts are on constrained control policies C^* and/or C_* over a time interval $\Delta t \subseteq T^0$, the exit conversion $X(1,t)$, corresponding to a non-varying inlet conversion $X_0(t)$ in time and resulting from an optimal operation, cannot be maintained constant in value over that time period, but is a continuous and monotonic decreasing function of time.

This is clearly demonstrated using the following result.

Property 6:

When at a particular time t parts of a reactor are on a stationary control policy S with other parts on constrained control policies C^* and/or C_* in time, the rate of change of exit conversion $X(1,t)$ in time where $X_0(t)$ is continuous differentiable is given by,

$$\frac{dX(1,t)}{dt} = \frac{\frac{F[X(1,t)]}{F[X_0(t)]} \cdot \frac{dX_0(t)}{dt} - \left(\frac{t_\theta}{t_f}\right).F[X(1,t)].\left\{K^*.k^*. \int_{\delta z_1(t)} g[\psi].dz + K_*.k_*. \int_{\delta z_2(t)} g[\psi].dz\right\}}{\{\, 1 - \beta. \int_{\delta z_0(t)} K^0(\varepsilon).\psi^0(\varepsilon).d\varepsilon \,\}}$$

with δz_0, δz_1, and δz_2 representing respectively length of the bed on control policies S, C^* and C_*.

Proof:

Integrating (3-31) at constant t from $z_o = 0$ to $z_f = 1$,

$$\int_{X_o(t)}^{X(1,t)} \frac{dY}{F[Y]} = (t_\Theta/t_f) \cdot \int_0^1 K(\varepsilon,t).\psi(\varepsilon,t) \cdot d\varepsilon \qquad (5\text{-}68)$$

Substituting (5-63) in (5-68) for the length δz_o where the reactor is on a control policy S,

$$\int_{X_o(t)}^{X(1,t)} \frac{dY}{F[Y]} = (t_\Theta/t_f).\left[\left\{\frac{F_1(t)}{F_1^o}\right\}^{\alpha}. \int_{\delta z_o(t)} K^o(\varepsilon).\psi^o(\varepsilon).d\varepsilon + K^*. \int_{\delta z_1(t)} \psi(\varepsilon,t).d\varepsilon + K_*. \int_{\delta z_2(t)} \psi(\varepsilon,t).d\varepsilon\right] \qquad (5\text{-}69)$$

and where δz_1 and δz_2 represent respectively lengths of the bed on control policies C^* and C_*. Differentiating (5-69) at constant z and with respect to t,

$$\frac{1}{F[X(1,t)]} \cdot \frac{dX(1,t)}{dt} - \frac{1}{F[X_o(t)]} \cdot \frac{dX_o(t)}{dt} \qquad (5\text{-}70)$$

$$= \left\{\frac{\beta}{F[X(1,t)]} \cdot \int_{\delta z_o(t)} K^o(\varepsilon).\psi^o(\varepsilon).d\varepsilon\right\} \cdot \frac{dX(1,t)}{dt} + \left(\frac{t_\Theta}{t_f}\right).K^* \int_{\delta z_1(t)} \frac{\partial\psi(\varepsilon,t)}{\partial t} .d\varepsilon +$$

$$+ \left(\frac{t_\Theta}{t_f}\right) \cdot K_* \cdot \int_{\delta z_2(t)} \frac{\partial\psi(\varepsilon,t)}{\partial t} \cdot d\varepsilon$$

with,

$$\beta = \frac{(t_\theta/t_f).\alpha.F'[X(1,t)].F_1^{\alpha}(t)}{(F_1^{o})^{\alpha}} \tag{5-71}$$

Rearranging (5-70) and using (3-31),

$$\frac{d\,X(1,t)}{dt}.\left\{1 - \beta \;.\int_{\delta z_o} K^{o}(\varepsilon).\psi^{o}(\varepsilon).\,d\,\varepsilon\right\} \tag{5-72}$$

$$= \frac{F[X(1,t)]}{F[X_o(t)]}.\frac{dX_o(t)}{dt} - (\frac{t_\theta}{t_f}).F[X(1,t)].\{K^{*}.k^{*}.\int_{\delta z_1} g[\psi].d\varepsilon + K_{*}.k_{*}.\int_{\delta z_2} g[\psi].d\,\varepsilon\}$$

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Therefore, since the results of the operations between braces on the right side of equation (5-72) are strictly positive, the exit conversion $X(1,t)$, corresponding to a continuous non-increasing inlet conversion $X_o(t)$ in time for all $t \in \Delta t \subset T$, is then a continuous and monotonic non-increasing function of time for all $t \in \Delta t$. By definition, $F[X(1,t)]$ is then a continuous and non-decreasing function of time there.

Now when the entire reactor bed is on a stationary control policy S, the following result holds.

Sub-Property 6a:

When the entire reactor is on a stationary control policy S in time, the rate of conversion $X(z,t)$ in time is given everywhere in the reactor by,

$$\frac{\partial X(z,t)}{\partial t} = \frac{F[X(z,t)]}{F[X_o(t)]} \cdot \left[\frac{1 - \beta \cdot \int_z^1 K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon}{1 - \beta \cdot \int_o^1 K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon} \right] \cdot \frac{dX_o(t)}{dt}$$

Proof:

Substituting (5-63) in (3-31) and integrating at constant t, from $z_o = 0$ to $z_f = z$,

$$\int_{X_o(t)}^{X(z,t)} \frac{dY}{F[Y]} = (t_\Theta / t_f) \cdot \left\{ \frac{F_1(t)}{F_1^o} \right\}^{\alpha} \cdot \int_o^z K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon \qquad (5\text{-}73)$$

Now differentiating (5-73) at constant z and with respect to t,

$$\frac{1}{F[X(z,t)]} \cdot \frac{\partial X(z,t)}{\partial t} - \frac{1}{F[X_o(t)]} \cdot \frac{d\,X_o(t)}{dt} = \left\{ \frac{\beta}{F[X(1,t)]} \cdot \int_o^z K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon \right\} \cdot \frac{d\,X(1,t)}{dt} \qquad (5\text{-}74)$$

with β given by (5-71).

Rearranging (5-74),

$$\frac{\partial X(z,t)}{\partial t} = \frac{F[X(z,t)]}{F[X_o(t)]} \cdot \frac{dX_o(t)}{dt} + \left\{\frac{\beta . F[X(z,t)]}{F[X(1,t)]} \cdot \int_o^z K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon\right\}.\frac{dX(1,t)}{dt} \tag{5-75}$$

Now for $z = 1$, equation (5-75) becomes,

$$\frac{dX(1,t)}{dt} = \frac{F[X(1,t)]/F[X_o(t)]}{\{1-\beta.\int_o^1 K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon\}} \cdot \frac{dX_o(t)}{dt} \tag{5-76}$$

Therefore when the entire bed is on a stationary control policy S, that is for all $z \in [o,1]$, substitution of (5-76) in (5-75) gives,

$$\frac{\partial X(z,t)}{\partial t} = \frac{F[X(z,t)]}{F[X_o(t)]} \cdot \left\{\frac{1-\beta.\int_z^1 K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon}{1-\beta.\int_o^1 K^o(\varepsilon).\psi^o(\varepsilon).d\,\varepsilon}\right\} \cdot \frac{dX_o(t)}{dt} \tag{5-77}$$

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Since the terms pre-multiplying $\frac{dX_o(t)}{dt}$ in equation (5-77) are strictly positive on a policy S, a major consequence of that result is that when the inlet conversion is a constant in time, the conversion everywhere in the reactor and resulting from such an extremal control policy is a constant in time for all $t \in \Delta t \subset T^o$.

When this is the case, the effective rate constant for reaction, expressed by (5-63), is a constant in time at each and every station $z \in [o,1]$.

In relation with these observations and those of property 6, the following results are obtained.

Property 7:

> When the inlet conversion $X_0(t)$ to the reactor is a continuous and monotonic non-increasing function of time, then an optimal control $k^+(z,t)$ defining a stationary policy S is a continuous and monotonic increasing function of time.

Proof:

Rewrite equation (5-63) in the form,

$$K(z,t) = \frac{\psi^0(z).K^0(z)}{(F_1{}^0)^\alpha} \cdot \frac{F_1{}^\alpha(t)}{\psi(z,t)} \qquad (5\text{-}78)$$

Now $F_1(t)$, with the stated assumptions on $X_0(t)$, is a continuous monotone non-decreasing function of time and $\psi(z,t)$ is a continuous monotonic decreasing function of time. Therefore, the rate constant $K(z,t)$ and thus $k(z,t)$, at each and every station $z \in [o,1]$ for which a stationary control exists, is a continuous monotone increasing function of time.

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Sub-Property 7a:

When the inlet conversion $X_o(t)$ to the reactor is a continuous and monotonic non-increasing function of time, then an optimal control policy $C^+(z,t)$ in time, may consist only of the following continuous and monotonic non-decreasing control policies in time:

Type I: $C^+ = \{C^*\}$ all $t \in [o,1]$

Type II: $C^+ = \begin{cases} S & t \in [o,t^*] \\ C^* & t \in [t^*,1] \end{cases}$

Type III: $C^+ = \begin{cases} C_* & t \in [o,t_*] \\ S & t \in [t_*,t^*] \\ C^* & t \in [t^*,1] \end{cases}$

at each and every station $z \in [o,1]$, where t^* and t_* are in general functions of z.

Proof:

Because of property 1, with the stated assumptions, an optimal control policy at any given station $z \in [o,1]$ must end on C^*, and,

$$\left.\frac{\partial H}{\partial k}\right|_{t=1} > 0 \qquad (5\text{-}79)$$

From equation (5-52), the time dependence of $(\frac{\partial H}{\partial k})$ for constant k(z,t) is given by:

$$\frac{\partial}{\partial t} \cdot (\frac{\partial H}{\partial k}) = \frac{1}{k^2} \cdot \{p.(\psi K) \cdot \frac{\partial F_1(t)}{\partial t} + (p-1).K.F_1(t) \cdot \frac{\partial \psi}{\partial t}\} \qquad (5\text{-}80)$$

Since conversion X(1,t) decreases with time at constant $k^+(z,t)$ and since $\frac{\partial \psi}{\partial t} < 0$, equation (5-80) implies that,

$$\frac{\partial}{\partial t} \cdot \left(\frac{\partial H}{\partial k}\right) > 0 \qquad (5\text{-}81)$$

Inequalities (5-79) and (5-81) indicate therefore that $\left(\frac{\partial H}{\partial k}\right)$ will decrease with decreasing time along a policy $k^+ = k^*$ from its positive value at t = 1.

A switch to a stationary policy S occurs if $\frac{\partial H}{\partial k}$ becomes zero before t = 0. Then because of property 7, with the given assumption, a switch from a policy S to a policy C_* occurs if the lower control limit k_* is reached before t = 0.

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When the inlet conversion $X_0(t)$ to the reactor is a continuous and monotonic increasing function of time but its rate of change is such that $\frac{\partial k^+}{\partial t} \geqslant 0$ there, then an optimal control policy C^+ in time also may consist only of a control policy of type I, II or III.

For continuous but arbitrary variations of $X_0(t)$ in time, these control policies are still principal ones to an optimal control policy C^+.

5.3.1. First-Order Catalyst Deactivation: [0 < p < 1]

If in equation (3-32) the function $g[\psi]$ assumes the power form:

$$g[\psi] = \psi^m \qquad (5\text{-}82)$$

with the order of deactivation m = 1 and if the control k(z,t) at any time $t \in \Delta t$ has a uniform value for all $z \in [o,1]$, then the activity $\psi(z,t)$ is characterized there by the fact that it can be expressed as a product of

separate functions (see Appendix D),

$$\psi(z,t) = \Psi_1(z) \cdot \Psi_2(t) \qquad \text{all } z \in [o,1],\ t \in \Delta t \qquad (5\text{-}83)$$

each of which depends only on z and t respectively. A consequence of that observation is given in the following result.

Property 8:

> For a first-order catalyst deactivation process when the inlet conversion $X_o(t)$ is continuous in time for $t \in [1-\delta t,1]$, $\delta t > 0$, and $\psi(z,1) \cdot F[X(1,1)] > 0$ for all $z \in [o,1]$, then any switch in control from a policy C^* to a policy S occurring at time $t_s \in (1-\delta t,1)$, $\delta t > 0$, occurs uniformly along the whole bed, that is for all $z \in [o,1]$, irrespective of the uniformity or continuity of the catalyst activity distribution there.

Proof:

Because of properties 1 and 2, with the stated assumptions, there exists a time $t \in [1-\delta t,1]$, $\delta t > 0$, such that everywhere in the reactor, the gradient (5-19) is strictly positive and,

$$k^+(z,t) = k^* \qquad \text{all } z \in [o,1] \qquad (5\text{-}84)$$

Since the control (5-84) has a uniform value for all $z \in [o,1]$ characteristic (5-83) applies and the gradient (5-19) with result (D-18) may be written,

$$\frac{\partial H}{\partial k} = \frac{\Psi_1(z)}{k^*} .\{p.F_1(t).K^*.\Psi_2(t) - k^*. \int_t^1 K^*.F_1(\varepsilon).\Psi_2(\varepsilon)\, d\,\varepsilon\} \qquad (5\text{-}85)$$

for all $z \in [o,1]$. Equation (5-85) consists of a product of separable terms each of which depends only on time t or distance z.

Therefore when the gradient (5-19) becomes identically zero at a time $t_s \in (1-\delta t,1)$ at a station $z \in [o,1]$, the strictly time-dependent term,

$$p.F_1(t).K^*.\Psi_2(t) - k^*. \int_{t_s}^1 K^*.F_1(\varepsilon).\Psi_2(\varepsilon).d\,\varepsilon = 0 \qquad (5\text{-}86)$$

is zero identically everywhere along the reactor length.

Since $\Psi_1(z) > 0$ by assumption, a simultaneous switch in control from a policy C^* to a policy S in time occurs uniformly over all $z \in [o,1]$.

Since no continuity or uniformity argument has been imposed on $\Psi_2(z)$ in this discussion, the result is general in that respect.

★

Sub-Property 8a:

> For a first-order catalyst deactivation process, an optimal control $k^+(z,t)$ in time $t \in [o,1]$ is uniform in value along the entire length of the reactor, that is for all $z \in [o,1]$, irrespective of the uniformity or continuity of the catalyst activity distribution along the length of the bed.

Proof:

It is shown in property 8 that for $t \in [t_s,1]$

$$\hat{k}(z,t) = k^* \qquad \text{all } z \in [o,1] \tag{5-87}$$

Since at $t = t_s$ a stationary control policy S is initiated for all $z \in [o,1]$, relation (5-63) holds there for $t \leqslant t_s$ and may be written for two different arbitrary stations z_1, $z_2 \in [o,1]$,

$$\psi(z_1,t).K(z_1,t) = \frac{\psi^o(z_1).K^o(z_1)}{(F_1{}^o)^\alpha}.F_1^\alpha(t) \tag{5-88}$$

$$\psi(z_2,t).K(z_2,t) = \frac{\psi^o(z_2).K^o(z_2)}{(F_1{}^o)^\alpha}.F_1^\alpha(t) \tag{5-89}$$

Choosing as a common reference time $t^o = t_s$ for the quantities ψ^o, K^o and $F_1{}^o$, the ratio of relations (5-88) and (5-89) gives:

$$\frac{\psi(z_1,t).K(z_1,t)}{\psi(z_2,t).K(z_2,t)} = \frac{\psi^o(z_1).K^o(z_1)}{\psi^o(z_2).K^o(z_2)} \tag{5-90}$$

For a first order catalyst deactivation process, the following relation (see Appendix D) is written for $t \leqslant t_s$:

$$\psi(z_i,t) = \psi(z_i,t_s).\ \exp\{+\int_t^{t_s} k(z_i,\delta).d\delta\} \qquad i = 1,2 \tag{5-91}$$

Recalling that with $t^o = t_s$, from (5-65),

$$\psi^o(z_i) = \psi(z_i,t_s) \qquad i = 1,2 \tag{5-92}$$

and that from (5-66) with (5-87),

$$K^o(z_i) = K(z_i,t_s) = K^* \qquad i = 1,2 \tag{5-93}$$

substitution of (5-91), (5-92) and (5-93) in (5-90) and rearranging:

$$K(z_1,t).\exp\{+\int_t^{t_s} k(z_1,\delta).d\delta\} = K(z_2,t).\exp\{+\int_t^{t_s} k(z_2,\delta).d\delta\} \quad (5\text{-}94)$$

In the equivalent logarithmic form,

$$\ln\{\frac{K(z_1,t)}{K(z_2,t)}\} = \int_t^{t_s} [k(z_2,\delta) - k(z_1,\delta)].d\delta \quad (5\text{-}95)$$

Now for $t = t_s - \delta t_s$ with δt_s arbitrarily chosen but $\delta t_s > 0$ and such that $t \in [o,t_s)$, assume that,

$$k(z_2,t) - k(z_1,t) > 0 \qquad \text{for all } t \in [t_s-\delta t_s, t_s) \quad (5\text{-}96)$$

Then since $K \alpha k^p$,

$$\ln\{\frac{K(z_1,t)}{K(z_2,t)}\} < 0 \qquad \text{for all } t \in [t_s-\delta t_s, t_s) \quad (5\text{-}97)$$

and relation (5-95) is violated there.

Assume again that,

$$k(z_2,t) - k(z_1,t) < 0 \qquad \text{for all } t \in [t_s-\delta t_s, t_s) \quad (5\text{-}98)$$

then,

$$\ln\{\frac{K(z_1,t)}{K(z_2,t)}\} > 0 \qquad \text{for all } t \in [t_s-\delta t_s, t_s) \quad (5\text{-}99)$$

and relation (5-95) is again violated there.

The only admissible proposition is then,

$$k(z_2,t) = k(z_1,t) \qquad \text{for all } t \in [t_s-\delta t_s, t_s) \qquad (5\text{-}100)$$

Therefore on an S policy, since z_1 and z_2 are arbitrarily chosen in $z \in [o,1]$, an extremal control $\hat{k}(z,t)$ at any time $t \leq t_s$ is uniform in value over all $z \in [o,1]$.

If a stationary policy S switches to a policy C_* before t = 0., the whole bed reaches $\hat{k}(z,t) = k_*$ uniformly there.

Since no continuity or uniformity argument has been imposed on $\psi(z,t)$ with respect to z, at any time $t \in [o,1]$, the result obtained is general in that respect.

★

5.4. $1 < p < \infty$

Raising the temperature when p > 1 would increase the rate constant K[T] for reaction faster than the rate constant k[T] for deactivation and would seem desirable.

However, although an increase in temperature everywhere over a finite length of the bed $\Delta z \subseteq Z^0$ would then increase the conversion $X(z,t)$ for all $z \in (z_s, z_s + \Delta z]$, $z_s \in [0,1]$, the rate of reaction could decrease because $F'[X(z,t)] \leqslant 0$.

Unless the reaction is zero order for which $F'[X(z,t)] = 0$ and so conversion does not affect the rate of reaction, a decrease of reaction rate through an increase of $X(z,t)$ could overweigh the increase through raising temperature.

At low conversion level increasing the temperature would increase the reaction rate relative to the decay rate with only a small decrease in $F[X(z,t)]$, but at higher conversions, however, raising the temperature may decrease $F[X(z,t)]$ more than the increase of $K[T]$ relative to $k[T]$. This would then suggest that the temperature should not be raised everywhere as high as possible.

Now for $p > 1$, the occurrence of a discontinuous control policy as an extremal control policy is possible and is established below.

Property 9:

When $\psi(z,t).F[X(1,t)] > 0$ for all $z,t \in \tau$, then a stationary control policy S is no longer an admissible control sub-policy in an extremal control policy.

Proof:

For $p > 1$, given that $\psi(z,t).F[X(1,t)] > 0$ for all $(z,t) \in \tau$, the second partial derivative (5-29),

$$\frac{\partial^2 H}{\partial k^2} > 0 \tag{5-101}$$

for all admissible control $k(z,t) \in [k_*, k^*]$ at each and every point $(z,t) \in \tau$ and constitutes a sufficient condition for the function H to be globally a minimum on a stationary control policy S. Clearly in this case, no stationary policy S may be a part of an extremal control policy.

★

Thus properties 2 and 9, with the stated assumptions, establish that at any given station of the reactor $z \in [o,1]$ an extremal control $\hat{k}(z,t)$ in time may only consist of control sub-policies C^* and C_* with a sub-policy C^* over a terminal time interval.

Conditions (5-17) and (5-18), however, represent only necessary conditions for a control to be extremal. Since the strict convexity of the function H with respect to controls k has been established in property 9, namely equation (5-101), typical curves of the function H with respect to $\hat{k} \in [k_*, k^*]$ are illustrated in figure 5-2. Sufficient conditions that a control must obey in order to be extremal at a control boundary k^* or k_* are:

$$\text{sgn} \left\{ \frac{\partial H}{\partial k} \bigg|_{k^*} \right\} = \text{sgn} \left\{ \frac{\partial H}{\partial k} \bigg|_{k_*} \right\} = \text{sgn} \{2.\hat{k}(z,t) - (k^* + k_*)\} \tag{5-102}$$

for $\hat{k}(z,t) = k^*$ or $\hat{k}(z,t) = k_*$.

These conditions are well identified for curves (a) and (c) of figure 5-2. In general, however, as illustrated for curve (b) of figure 5-2, conditions (5-102) need not be necessarily satisfied for a control to be extremal at a control boundary k^* or k_*. Admissible extremal control candidates in the following are discriminated using the global condition (4-16):

$$\Delta H(z,t) = \left\{ H(z,t) - \bar{H}(z,t) \right\} \geq 0 \tag{5-103}$$

where at each and every point $(z,t) \in \tau$, from (D-27),

$$H(z,t) = \psi . F_1 . \hat{K} - \hat{k} . \int_t^1 \hat{K} . F_1 . \, g[\psi] . d\,\delta \tag{5-104}$$

and

$$\bar{H}(z,t) = \psi . F_1 . \bar{K} - \bar{k} . \int_t^1 \hat{K} . F_1 . \, g[\psi] . d\,\delta \tag{5-105}$$

where $\hat{k} = \hat{k}(z,t)$ represents the extremal control from time $t = t$ to $t = 1$ and $\bar{k} = \bar{k}(z,t)$ is the other admissible control candidate at any time t. The state variables $\psi(z,t)$ and $X(1,t)$, thus $F_1(t)$, are the solutions to equations (3-32) and (3-31) and their respective initial and boundary conditions (3-35) and (3-33) obtained from time $t = t$ to $t = 1$ and for all $z \in [o,1]$ using the control $\hat{k}(z,t)$.

Consideration of properties 1 and 2 with the stated assumptions there, shows that sufficient conditions (5-102) are satisfied with $\hat{k}(z,t) = k^*$ at each and every station $z \in [o,1]$, and

$$\Delta H(z,t) > 0 \tag{5-106}$$

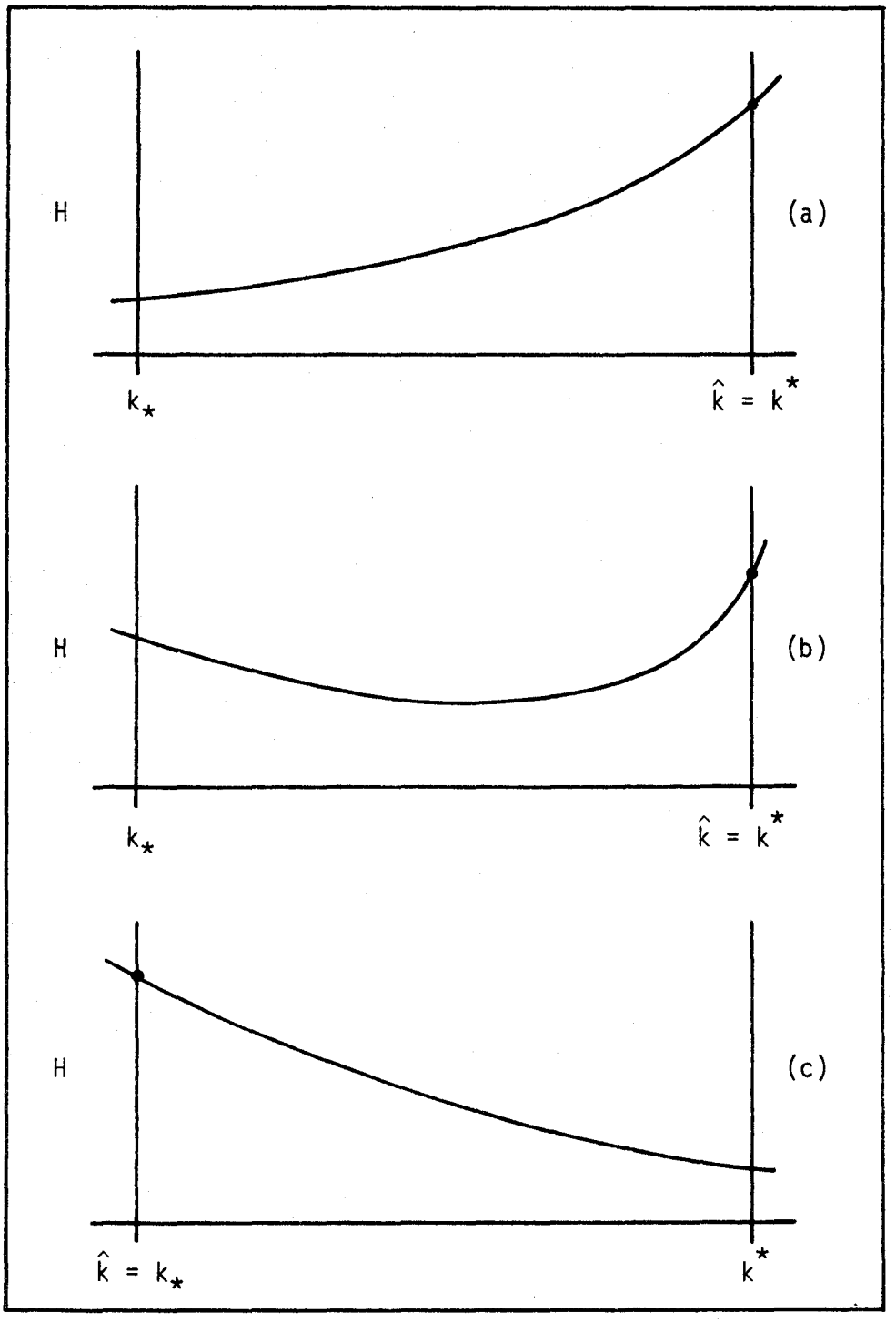

Figure 5-2 Typical Curves Of The Function H(z,t) Versus The Control $k_* \leq k(z,t) \leq k^*$ for $1 < p < \infty$.

there, with

$$\Delta H(z,t) = \psi.F_1.\Delta K - \Delta k.\int_t^1 K^*.F_1.\, g[\psi].d\,\delta \qquad (5\text{-}107)$$

$$\Delta K = (K^* - K_*) > 0 \qquad (5\text{-}108)$$

$$\Delta k = (k^* - k_*) > 0 \qquad (5\text{-}109)$$

Because conditions (5-102) are sufficient but not necessary for $\hat{k}(z,t) = k^*$, there may exist corresponding to each and every station $z \in [o,1]$ a time interval $\delta t > \delta t_1 \geqslant \delta t_o$, where $X_o(t)$ is continuous, such that for all points $(z,t) \in Z^o \times (1-\delta t_1, 1]$, $\hat{k}(z,t) = k^*$ and that condition (5-103) is true.

Therefore the function $\Delta H(z,t)$ at each and every station $z \in [o,1]$ is a continuous function of time and has a continuous first partial derivative everywhere with respect to time $t \in (1-\delta t_1, 1]$ except possibly for a set of points on δt_1, namely at the points of discontinuity of $\frac{dX_o(t)}{dt}$, where it may have a discontinuity of the first kind.

On intervals of time for which,

$$\frac{\partial \Delta H(z,t)}{\partial t} = \frac{\partial H(z,t)}{\partial t} - \frac{\partial \bar{H}(z,t)}{\partial t} \qquad (5\text{-}110)$$

is continuously defined, equation (5-104) becomes with $\hat{K} = K^*$ and $\hat{k} = k^*$,

$$\frac{\partial H(z,t)}{\partial t} = F_1.K^*.\frac{\partial \psi}{\partial t} + F_1'.\psi.K^*.\frac{dX(1,t)}{dt} + k^*.K^*.F_1.g[\psi] \qquad (5\text{-}111)$$

recalling (3-32) with $\hat{k} = k^*$,

$$\frac{\partial H(z,t)}{\partial t} = F_1'.\psi.K^*.\frac{dX(1,t)}{dt} \tag{5-112}$$

Similarly for equation (5-105) with $\bar{K} = K_*$ and $\bar{k} = k_*$,

$$\frac{\partial \bar{H}(z,t)}{\partial t} = F_1.K_*.\frac{\partial \psi}{\partial t} + F_1'.\psi.K_*.\frac{dX(1,t)}{dt} + k_*.K^*.F_1.g[\psi] \tag{5-113}$$

and (3-32) with $\hat{k} = k^*$,

$$\frac{\partial \bar{H}(z,t)}{\partial t} = F_1'.\psi.K_*.\frac{dX(1,t)}{dt} + F_1.\ g[\psi].\ \Delta(Kk) \tag{5-114}$$

with,

$$\Delta(Kk) = K^*.k_* - K_*.k^* \tag{5-115}$$

and since by (3-37) $K = A.k^p$, and for $p > 1$,

$$\Delta(Kk) = A.k^*.k_*.\{k^{*p-1} - k_*^{p-1}\} > 0 \tag{5-116}$$

Finally, equation (5-110) may be written,

$$\boxed{\frac{\partial \Delta H(z,t)}{\partial t} = F_1'.\psi.\Delta K.\frac{dX(1,t)}{dt} - F_1.g[\psi].\Delta(Kk)} \tag{5-117}$$

with ΔK defined in (5-108).

The case of a zero order reaction is treated below and it is shown that an optimal control policy everywhere in τ may only be purely C^*.

Property 10:

> For $\psi(z,1) > 0$ an optimal control policy corresponding to a zero order reaction may consist only of,
>
> $$k^{+}(z,t) = k^{*} \qquad \text{all } (z,t) \in \tau$$
>
> that is a pure control policy C^{*} in the whole of τ.

Proof:

Since for a zero order reaction $F[X(1,t)]$ is a positive constant, $F_1' = 0$ and equation (5-117) reduces to,

$$\frac{\partial \Delta H(z,t)}{\partial t} = - g[\psi] \cdot F_1 \cdot \Delta(Kk) \tag{5-118}$$

Recalling property 1, with the stated assumption, function (5-107) with $k^{+}(z,1) = k^{*}$ for all $z \in [o,1]$ may be written,

$$\Delta H(z,1) = \psi(z,1) \cdot F_1 \cdot \Delta K > 0 \tag{5-119}$$

with ΔK given by (5-108). Since by (5-116) $\Delta(Kk)$ is strictly positive and since the catalyst activity is a continuous and monotonic decreasing function of time, then with the stated assumption, $\psi(z,t) > 0$ for all $(z,t) \in \tau$, and relation (5-118) becomes,

$$\frac{\partial \Delta H(z,t)}{\partial t} < 0 \qquad \text{for all } (z,t) \in \tau \tag{5-120}$$

Therefore, since $\Delta H(z,1) > 0$ for all $z \in [o,1]$, the function $\Delta H(z,t)$,

because of (5-120), will always be positive everywhere in τ and the maximum condition (5-106) will be satisfied there for $k^{+}(z,t) = k^{*}$.

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Therefore, unless a reaction is zero order, the rate of change of the function $\Delta H(z,t)$ with time may be positive for some finite intervals of time. Accordingly, since the function $\Delta H(z,t)$ is positive at $t = 1$ it could decrease in value with decreasing time and could possibly reach a value zero at some time $t_s \in (1-\delta t_1, 1]$.

When this is the case, the function $\Delta H(z,t_s)$ at a time $t_s \in (1-\delta t_1, 1]$ may become identically zero at one or many isolated stations $z \in [o,1]$ or uniformly zero along a finite length $\Delta z \subseteq [o,1]$ of the reactor. Also since the rate (5-117) would be positive at time t_s at these particular stations, a jump in control from a policy C^{*} to a policy C_{*} at one or more of these stations would need to be actuated at time $t = t_s^{-}$, otherwise the rate of change of $\Delta H(z,t)$ could remain positive there and the maximum condition be violated at these stations for $t < t_s$.

Although the maximum condition indicates that a jump in control from a policy C^{*} to a policy C_{*} may occur in an optimal sense at a time $t_s \in (1-\delta t_1, 1]$ when the null condition,

$$\Delta H(z,t_s) = 0 \qquad z \in [o,1] \tag{5-121}$$

exists at these stations, it does not insure however that a jump in control must be actuated at each of these stations.

The case where the null condition (5-121) exists at a time t_s but uniformly along a finite length of the reactor is investigated below and the results are summarized in the following property.

Property 11:

> When $X_o(t)$ is continuous in time for $t \in [t_1,t_2]$ and when the function $\Delta H(z,t)$ reaches a zero value at a time $t_s \in (t_1,t_2)$ but uniformly along a finite length $\Delta z \subseteq [o,1]$, a uniform jump in control occurring simultaneously along a finite length $\delta z \subseteq \Delta z$ is not optimal.

Proof:

Since at time t_s, $\hat{k}(z,t_s) = \hat{k}(\bar{z},t_s) = k^*$ and that,

$$\Delta H(\bar{z},t_s) = 0 \qquad \bar{z} \in \Delta z \qquad (5\text{-}122)$$

$$\Delta H(z,t_s) > 0 \qquad z \in \{Z^o \setminus \Delta z\} \qquad (5\text{-}123)$$

assume that a uniform switch in control along a finite length $\delta z \subseteq \Delta z$ is optimal,

$$\hat{k}(\hat{z},t_{\bar{s}}) = k_* \qquad \hat{z} \in \delta z \qquad (5\text{-}124)$$

where

$$t_{\bar{s}} = \text{limit}\{t_s - \delta t_s\} \qquad (5\text{-}125)$$

$$\delta t_s \to 0$$

$$\delta t_s > 0$$

then the function $H(\hat{z},t_{\bar{s}})$ and $\bar{H}(\hat{z},t_{\bar{s}})$ may be written there,

$$H(\hat{z},t_{\bar{s}}) = \{\psi(\hat{z},t_{\bar{s}}).F_1(t_{\bar{s}}).K_* - k_*.[\int_{t_s}^{1} K^*F_1 g \, d\delta + \int_{t_{\bar{s}}}^{t_s} K_*F_1 \, g \, d \, \delta]\} \quad (5\text{-}126)$$

with

$$\bar{H}(\hat{z},t_{\bar{s}}) = \{\psi(\hat{z},t_{\bar{s}}).F_1(t_{\bar{s}}).K^* - k^*.[\int_{t_s}^{1} K^*F_1 g \, d\delta + \int_{t_{\bar{s}}}^{t_s} K_*F_1 g \, d \, \delta]\} \quad (5\text{-}127)$$

and finally:

$$\Delta H(\hat{z},t_{\bar{s}}) = - \{\psi(\hat{z},t_{\bar{s}}).F_1(t_{\bar{s}}).\Delta K - \Delta k.[\int_{t_s}^{1} K^*F_1 g \, d\delta + \int_{t_{\bar{s}}}^{t_s} K_*F_1 g \, d \, \delta]\} \quad (5\text{-}128)$$

with ΔK and Δk given respectively by (5-108) and (5-109). Corresponding at time t_s,

$$\Delta H(\hat{z},t_s) = \{\psi(\hat{z},t_s).F_1(t_s).\Delta K - \Delta k. \int_{t_s}^{1} K^*F_1 \, g \, d \, \delta\} = 0 \quad (5\text{-}129)$$

substituting in equation (5-128),

$$\Delta H(\hat{z},t_{\bar{s}}) = - \{[\psi(\hat{z},t_{\bar{s}}).F_1(t_{\bar{s}}) - \psi(\hat{z},t_s).F_1(t_s)].\Delta K - \Delta k.\int_{t_{\bar{s}}}^{t_s} K_*F_1 g \, d \, \delta\} \quad (5\text{-}130)$$

The exit conversion at time t_s^- may be expressed as (see Appendix D),

$$X(1,t_s^-) = P[X_o(t_s^-),\ K_* \int_{\delta z_2} \psi(\varepsilon,t_s^-)\ d\varepsilon + K^* \int_{Z^o \setminus \delta z_2} \psi(\varepsilon,t_s^-).d\ \varepsilon] \qquad (5\text{-}131)$$

and at time t_s by,

$$X(1,t_s) = P[X_o(t_s),\ K^* \int_0^1 \psi(\varepsilon,\ t_s).d\ \varepsilon] \qquad (5\text{-}132)$$

Since the inlet conversion $X_o(t)$ and the relative activity everywhere in the reactor are both continuous functions of time, at the limit $t_s^- \to t_s$,

$$\psi(\hat{z},t_s^-) = \psi(\hat{z},t_s) \qquad (5\text{-}133)$$

$$X_o(t_s^-) = X_o(t_s) \qquad (5\text{-}134)$$

$$\int_{t_s^-}^{t_s} K_* F_1\ g.d\ \delta = 0 \qquad (5\text{-}135)$$

and expression (5-131) is rewritten there,

$$X(1,t_s^-) = P[\ X_o(t_s),\ K_* \int_{\delta z_2} \psi(\varepsilon,t_s).d\ \varepsilon + K^* \int_{Z^o \setminus \delta z_2} \psi(\varepsilon,t_s).d\ \varepsilon] \qquad (5\text{-}136)$$

Now since the integral of a positive quantity over a non-zero length δz_2 is a non-zero quantity, relations (5-136) and (5-132) indicate that, at the limit for (5-125),

$$X(1,t_s^-) < X(1,t_s) \qquad (5\text{-}137)$$

and that for a non-zero order reaction,

$$F_1(t_{\bar{s}}) > F_1(t_s) \tag{5-138}$$

Since substitution of results (5-133) and (5-134) in equation (5-130) gives,

$$\Delta H(\hat{z},t_{\bar{s}}) = \psi(\hat{z},t_s).\Delta K.\ \{F_1(t_s) - F_1(t_{\bar{s}})\} \tag{5-139}$$

and at the limit for $t_{\bar{s}}$ considering result (5-138),

$$\Delta H(\hat{z},t_{\bar{s}}) < 0 \tag{5-140}$$

Thus result (5-140) violates the maximum condition for all $\hat{z} \in \delta z_2$ where δz_2 is finite, and assumption (5-124) cannot be validated there.

In this proof, the allowable control jump is from a policy C^* to a policy C_* in decreasing time. The same result could be shown to be true if the allowable control jump was from a policy C_* to a policy C^* in decreasing time.

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Since jumps in control along a line parallel to the flow axis of the reactor are not optimal, conversion $X(z,t)$ at each and every station $z \in [o,1]$ corresponding to a continuous inlet conversion $X_o(t)$ in time and also resulting from the application of an extremal control policy there may only be a continuous function of time (see Appendix D).

This situation would suggest that jumps in control from a policy C^* to a policy C_* may only occur at time $t_{\bar{s}}$ at one or more isolated stations $z_s \in \Delta z$ at which $\Delta H(z_s,t_s) = 0$.

Recalling that an isolated station $z_s \in [o,1]$ has a length of measure zero and that the integral of an integrable function over a length of measure zero is zero, then in particular the contribution of the integral of the function $\{K_*.\psi(z,t)\}$ over lengths of measure zero to the integral,

$$\int_o^1 K(\varepsilon,t).\psi(\varepsilon,t)\, d\,\varepsilon \tag{5-141}$$

at any time t is nil and in the context of the proof of property 10, relation (5-131) could be written for that case:

$$X(1,t_s^-) = P[X_o(t_s^-),\ K^* \int_o^1 \psi(\varepsilon,t_s^-).\, d\,\varepsilon] \tag{5-142}$$

A consequence is that at the limit as $t_s^- \to t_s$, relations (5-137) and (5-138) would then become equalities and the maximum condition would be satisfied there at each and every of the stations $z_s \in \Delta z$ where a jump in control occurred.

Necessary and sufficient conditions that guarantee the maximum condition be satisfied for $t < t_s$ and all $z \in [o,1]$ are given below for the case where a jump in control has been initiated at time t_s^- at one or more isolated stations $z_s \in \Delta z \subseteq Z^o$.

Consider a jump in control such that at a station $z_s \in \Delta z$,

$$\hat{k}(z_s,t) = k_* \tag{5-143}$$

for $t < t_s$.

The function $\Delta H(z_s,t)$ given in (5-107) is then written,

$$\Delta H(z_s,t) = - \{\psi(z_s,t).F_1(t).\Delta K - \Delta k. \left[\int_{t_s}^{1} K^* F_1 g \, d\delta + \int_{t}^{t_s} K_* F_1 g \, d\delta \right]\} \quad (5\text{-}144)$$

which can also be written (see Appendix E),

$$\Delta H(z_s,t) = + \int_{t}^{t_s} \left[\psi(z_s,\delta).F_1'(\delta). \frac{dX(1,\delta)}{d\delta} .\Delta K - F_1(\delta).g[\psi].\Delta(Kk)\right] d\delta \quad (5\text{-}145)$$

$$+ \Delta H(z_s,t_{\bar{s}})$$

with ΔK, Δk and $\Delta(Kk)$ given respectively by (5-108), (5-109) and (5-115). Since $X(1,t)$ is a continuous function of time and given that a jump in control has occurred at $t_{\bar{s}}$, then at the limit for $t_{\bar{s}} \to t_s$,

$$\Delta H(z_s,t_{\bar{s}}) = - \Delta H(z_s,t_s) \quad (5\text{-}146)$$

and since $\Delta H(z_s,t_s) = 0$. by assumption, a necessary and sufficient condition for $\Delta H(z_s,t) \geqslant 0$ for all $z_s \in \Delta z$ and all $t < t_s$ where control (5-136) holds is given by (5-145):

$$\boxed{\int_{t}^{t_s} \left[\psi(z_s,\delta).F_1'(\delta). \frac{dX(1,\delta)}{d\delta} .\Delta K - F_1(\delta).g[\psi].\Delta(Kk)\right] d\delta \geqslant 0} \quad (5\text{-}147)$$

Now consider other stations $\bar{z} \in \Delta z$ but $\bar{z} \neq z_s$ for which a jump in control has not yet occurred at a time $t < t_s$, that is,

$$\hat{k}(\bar{z},t) = k^* \tag{5-148}$$

The function $\Delta H(\bar{z},t)$ is then written, using (5-107),

$$\Delta H(\bar{z},t) = + \{\psi(\bar{z},t).F_1(t).\Delta K - \Delta k.[\int_{t_s}^{1} K^* F_1 \, g \, d\delta + \int_{t}^{t_s} K^* F_1 \, g \, d\,\delta]\} \tag{5-149}$$

or in the form (see Appendix E),

$$\Delta H(\bar{z},t) = - \int_{t}^{t_s} [\psi(\bar{z},\delta).F_1'(\delta).\frac{dX(1,\delta)}{d\delta}.\Delta K - F_1(\delta).g[\psi].\Delta(Kk)].d\,\delta + \Delta H(\bar{z},t_{\bar{s}}) \tag{5-150}$$

with ΔK, Δk and $\Delta(Kk)$ given as before. Since $X(1,t)$ is a continuous function of time and that no jump in control has occurred at $t_{\bar{s}}$, at the limit for $t_{\bar{s}} \to t_s$,

$$\Delta H(\bar{z},t_{\bar{s}}) = + \Delta H(\bar{z},t_s) \tag{5-151}$$

Also because $\Delta H(\bar{z},t_s) = 0$. by assumption, a necessary and sufficient condition for $\Delta H(\bar{z},t) \geq 0$ for all $\bar{z} \in \Delta z$ but $\bar{z} \neq z_s$ and $t < t_s$ where control (5-148) holds is given by (5-150),

$$\boxed{\int_{t}^{t_s} [\psi(\bar{z},\delta).F_1'(\delta).\frac{dX(1,\delta)}{d\delta}.\Delta K - F_1(\delta).g[\psi].\Delta(Kk)].d\,\delta \leq 0} \tag{5-152}$$

If a jump in control need be actuated at a time $t_{sw} < t_s$ at any station $\bar{z} \in \Delta z$ but $\bar{z} \neq z_s$, the condition,

$$\Delta H(\bar{z},t_{sw}) = 0 \tag{5-153}$$

must be satisfied at this point and relation (5-152) becomes,

$$\int_{t_{sw}}^{t_s} [\psi(\bar{z},\delta).F_1'(\delta).\frac{dX(1,\delta)}{d\delta}.\Delta K - F_1(\delta).g[\psi].\Delta(Kk)].d\,\delta = 0 \tag{5-154}$$

Finally for stations $\hat{z} \in \{Z^o \backslash \Delta z\}$ at which the condition,

$$\Delta H(\hat{z},t_s) > 0 \tag{5-155}$$

exists and for which a jump in control at time $t < t_s$ has not yet occurred, that is,

$$\hat{k}(\hat{z},t) = k^* \tag{5-156}$$

the function $\Delta H(\hat{z},t)$ may be written there, using (5-107),

$$\Delta H(\hat{z},t) = + \{\psi(\hat{z},t).F_1(t).\Delta K - \Delta k.[\int_{t_s}^{1} K^* F_1\, g\, d\,\delta + \int_{t}^{t_s} K^*\, F_1\, g\, d\,\delta]\} \tag{5-157}$$

or equivalently in the form (see Appendix E),

$$\Delta H(\hat{z},t) = -\int_{t}^{t_s} [\psi(\hat{z},\delta).F_1'(\delta).\frac{dX(1,\delta)}{d\delta}.\Delta K - F_1(\delta).g[\psi].\Delta(Kk)].d\,\delta + \Delta H(\hat{z},t_s^-) \tag{5-158}$$

Because of the continuity of $X(1,t)$ and since no jump in control has occurred at t_s^-, at the limit for $t_s^- \to t_s$,

$$\Delta H(\hat{z},t_s^-) = +\Delta H(\hat{z},t_s) \tag{5-159}$$

However, because of condition (5-155) a necessary and sufficient condition for $\Delta H(\hat{z},t) \geq 0$ for all $z \in \{Z^0 \setminus \Delta z\}$ and all $t < t_s$ where control (5-156) holds is given by (5-158):

$$\boxed{\Delta H(\hat{z},t_s) - \int_{t}^{t_s} [\psi(\hat{z},\delta).F_1'(\delta).\frac{dX(1,\delta)}{d\delta}.\Delta K - F_1(\delta).g[\psi].\Delta(Kk)].\,d\,\delta \geq 0} \tag{5-160}$$

Similarly, if a jump in control need be actuated at a time $t_{sw} < t_s$ at any of these station $\hat{z}$, the condition,

$$\Delta H(\hat{z},t_{sw}) = 0 \tag{5-161}$$

must be satisfied at this point and (5-160) becomes,

$$\Delta H(\hat{z},t_s) - \int_{t_{sw}}^{t_s} [\psi(\hat{z},\delta).F_1'(\delta).\frac{dX(1,\delta)}{d\delta}.\Delta K - F_1(\delta).g[\psi].\Delta(Kk)].d\,\delta = 0 \quad (5\text{-}162)$$

In summary, for $p > 1$, unless a reaction is zero order for which an extremal control policy is purely C^* everywhere in τ, an extremal control in time may only consist at each and every station $z \in [o,1]$ of control sub-policies C^* and C_* with a sub-policy C^* over a terminal time interval. When the null condition $\Delta H(z,t) = 0$ is satisfied for $(z,t) \in \tau$ a possibility of a jump in control exists. It has been shown that when $\Delta H(z,t) = 0$ uniformly over a finite length of the reactor $\Delta z \subseteq Z^o$ a simultaneous jump in control along a finite length of the reactor $\delta z \subseteq \Delta z$ in time is not optimal. That is no control switching line in τ may be parallel to the flow axis of the reactor. It has also been indicated that a control switching line may be initiated at a time $t = t_s$ only at isolated points z_s where at a time $t_s \in (o,1)$ $\Delta H(z,t) = 0$ whether or not the null condition exists only at isolated points $z_s \in [o,1]$ or uniformly along a finite length of the bed $\Delta z \subseteq Z^o$ in which case $z_s \in \Delta z$.

Therefore, corresponding to each and every station $z \in [o,1]$, a jump in control may occur at a time $t_{sw}(z) < t_s$ defined implicitly by condition (5-154) for $z \in \Delta z$ and by condition (5-162) for $z \in (Z^o \backslash \Delta z)$ and a control switching line $w(z,t_{sw})$ may be traced out there for $(z,t) \in Z^o \times [o,t_s)$.

5.4.1. First Order Catalyst Deactivation [$1 < p < \infty$]

For time $t \geq t_s$ where a jump in control has not yet been initiated everywhere in $z \in [0,1]$, the control

$$\hat{k}(z,t) = k^* \tag{5-163}$$

is uniformly distributed for all points $(z,t) \in [0,1] \times [t_s,1]$. Recalling with equations (5-82) and (5-83) that for a first order catalyst deactivation process acting there, the catalyst activity may be expressed as a product of separate functions,

$$\psi(z,t) = \Psi_1(z).\Psi_2(t) \tag{5-164}$$

each of which depends only on z and t respectively, the function $\Delta H(z,t)$ given by (5-107) may be written there,

$$\Delta H(z,t) = \Psi_1(z).\left\{\Psi_2(t).F_1(t).\Delta K - \Delta k.\int_t^1 K^*.F_1(\delta).\Psi_2(\delta)d\delta\right\} \tag{5-165}$$

for all $z \in [0,1]$ and $t \geq t_s$. Since $\Psi_1(z) > 0$ by assumption, and noting that the expression inside the parenthesis of (5-165) is solely a function of time t, then if it reaches a value zero at a time t_s, it reaches it uniformly along the whole reactor, that is for all $z \in [0,1]$, irrespective of the quality of the catalyst distribution in the reactor $\Psi_1(z)$.

Therefore for a first order catalyst deactivation process, the condition,

$$\Delta H(z,t_s) = 0 \tag{5-166}$$

exists uniformly over the whole reactor, that is for all $z \in [0,1]$ at $t = t_s$. Hence $\Delta z = [0,1]$ and, with respect to property 11, a jump in control from a policy C^* to a policy C_* may only occur at time t_s at one or more isolated stations $z_s \in \Delta z$.

Necessary and sufficient conditions for controls to be extremal in time $t < t_s$ at stations $z_s \in \Delta z$ and $\bar{z} \in \Delta z$, but $\bar{z} \neq z_s$, are given in relations (5-147), (5-152) and (5-154). However for a catalyst deactivation process described by (3-32) and,

$$g[\psi] = \psi \tag{5-167}$$

conditions (5-147), (5-152) and (5-154) reduce to a strictly time dependent necessary and sufficient condition that an extremal control must obey for $t < t_s$ and all $z \in [0,1]$. This is indicated in the following property.

Property 12:

When the inlet conversion $X_o(t)$ is continuous in time for $t \in [t_1,t_2]$ and when the function $\Delta H(z,t)$, for a first order catalyst deactivation process, reaches a value zero uniformly along the whole reactor at time $t_s \in (t_1,t_2)$, then the condition,

$$F_1'(t).\frac{dX(1,t)}{dt}.\Delta K - F_1(t).\Delta(Kk) = 0.$$

constitutes a necessary and sufficient condition that must be obeyed by discontinuous control policies in the plane of $Z^o \times \Delta t = [0,1] \times (t_1,t_s)$ in order to satisfy the maximum condition there.

Proof:

Because of (5-167), relation (5-147), (5-152) and (5-154) may be written respectively:

$$\int_t^{t_s} \psi(z_s,\delta).Q(\delta).d\delta \geqslant 0 \qquad (5\text{-}168)$$

$$\int_t^{t_s} \psi(\bar{z},\delta).Q(\delta).d\delta \leqslant 0 \qquad (5\text{-}169)$$

$$\int_{t_{sw}}^{t_s} \psi(\bar{z},\delta).Q(\delta).d\delta = 0 \qquad (5\text{-}170$$

with

$$Q(t) = F_1^{*}(t).\frac{dX(1,t)}{dt}.\Delta K - F_1(t).\Delta(Kk) \qquad (5\text{-}171)$$

Now for $t = t_s - \delta t_s$ with δt_s arbitrarily chosen, but $\delta t_s > 0$ and such that $t \in (t_1,t_s)$, assume that,

$$Q(t) > 0 \qquad \text{for all } t \in [t_s-\delta t_s,t_s) \qquad (5\text{-}172)$$

since, by assumption, $\psi(z,t) > 0$ for all $z,t \in \tau$, then condition (5-168) is satisfied but condition (5-169) is violated there. Assume again that,

$$Q(t) < 0 \qquad \text{for all } t \in [t_s-\delta t_s,t_s) \qquad (5\text{-}173)$$

similarly, condition (5-172) is satisfied but condition (5-169) is violated there. The only admissible value is then,

$$Q(t) = 0 \qquad \text{for all } t \in [t_s-\delta t_s,t_s) \qquad (5\text{-}174)$$

and condition (5-168) and (5-169) become identically satisfied with the equality sign for all $t \in [t_s-\delta t_s,t_s)$.

Since the process of choosing δt_s is arbitrary and may be achieved for anytime, $t = \{t_s - \delta t_s\} \varepsilon (t_1, t_s)$, $\delta t_s > 0$, condition (5-174) must be satisfied at all time t there. Therefore condition (5-170) is also satisfied there for all $t_{sw} \varepsilon (t_1, t_s)$. Satisfying conditions (5-147), (5-152) and (5-154), equation (5-177), with Q(t) defined in (5-171), is a necessary and sufficient condition to be obeyed by discontinuous control policies in $Z^o \times \Delta t = [0,1] \times (t_1, t_s)$.

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A consequence of property 12 for first-order catalyst deactivation process is that extremal controls distributed everywhere in the reactor and thus satisfying condition (5-174) for time $t < t_s$ render function (5-107),

$$\Delta H(z,t) = 0 \tag{5-175}$$

identically zero for all $z \varepsilon [0,1]$ and $t < t_s$. This result (5-175) indicates the possibility of a jump in control at each and every point z,t there, and the problem of synthesizing extremal control policies in time $t < t_s$ at each and every station $z \varepsilon [0,1]$ would seem a formidable task. Fortunately, however, since condition (5-174) with (5-171) may be written,

$$\frac{d \ln F[X(1,t)]}{dt} = \frac{\Delta(Kk)}{\Delta K} \tag{5-176}$$

or more explicitly, integrating from time $t < t_s$ to time $t = t_s$,

$$\ln F[X(1,t)] \Big|_{t}^{t_s} = \frac{\Delta(Kk)}{\Delta K} .(t_s - t) \tag{5-177}$$

and involves the exit conversion $X(1,t)$ as an explicit function of time, it indicates that at any given time $t < t_s$, controls along the reactor length could be adjusted in order that, corresponding to an inlet conversion $X_0(t)$, the exit conversion,

$$X(1,t) = P[X_0(t), K^* \int_{\delta z_1} \psi(\varepsilon,t).d\varepsilon + K_* \int_{\delta z_2} \psi(\varepsilon,t).d\varepsilon] \qquad (5\text{-}178)$$

resulting from such action satisfies (5-177). In relation (5-178), δz_1 and δz_2 represent parts of the bed on a policy C^* and policy C_* respectively which could be varied continuously in time.

At time $t = t_s$, $\hat{k}(z,t_s) = k^*$ everywhere in the reactor and $\delta z_1 = [0,1]$ with $\delta z_2 = 0$. In order to satisfy relation (5-177) for $t < t_s$ some parts of the bed could need be on a C_* policy and $\delta z_2 \neq 0$ there.

Even if for $t < t_s$ this is the case and the integral quantity,

$$K^*. \int_{\delta z_1} \psi(\varepsilon,t).d\varepsilon + K_*. \int_{\delta z_2} \psi(\varepsilon,t).d\varepsilon \qquad (5\text{-}179)$$

must be related through relation (5-178), with a known inlet conversion $X_0(t)$, to a value given in time by (5-177), nothing is implied, however, about which portions of the actual bed need be the constitutive parts of δz_1 and δz_2.

Therefore for $t < t_s$, relation (5-178) may correspond to a value of $X(1,t)$ in time given by (5-177) and lead to more than one extremal control surface in τ. This situation is illustrated in figure 5-3 where two different extremal control surfaces are considered and may be constructed in order that for $t < t_s$, $X(1,t)$ be identical in value for both cases.

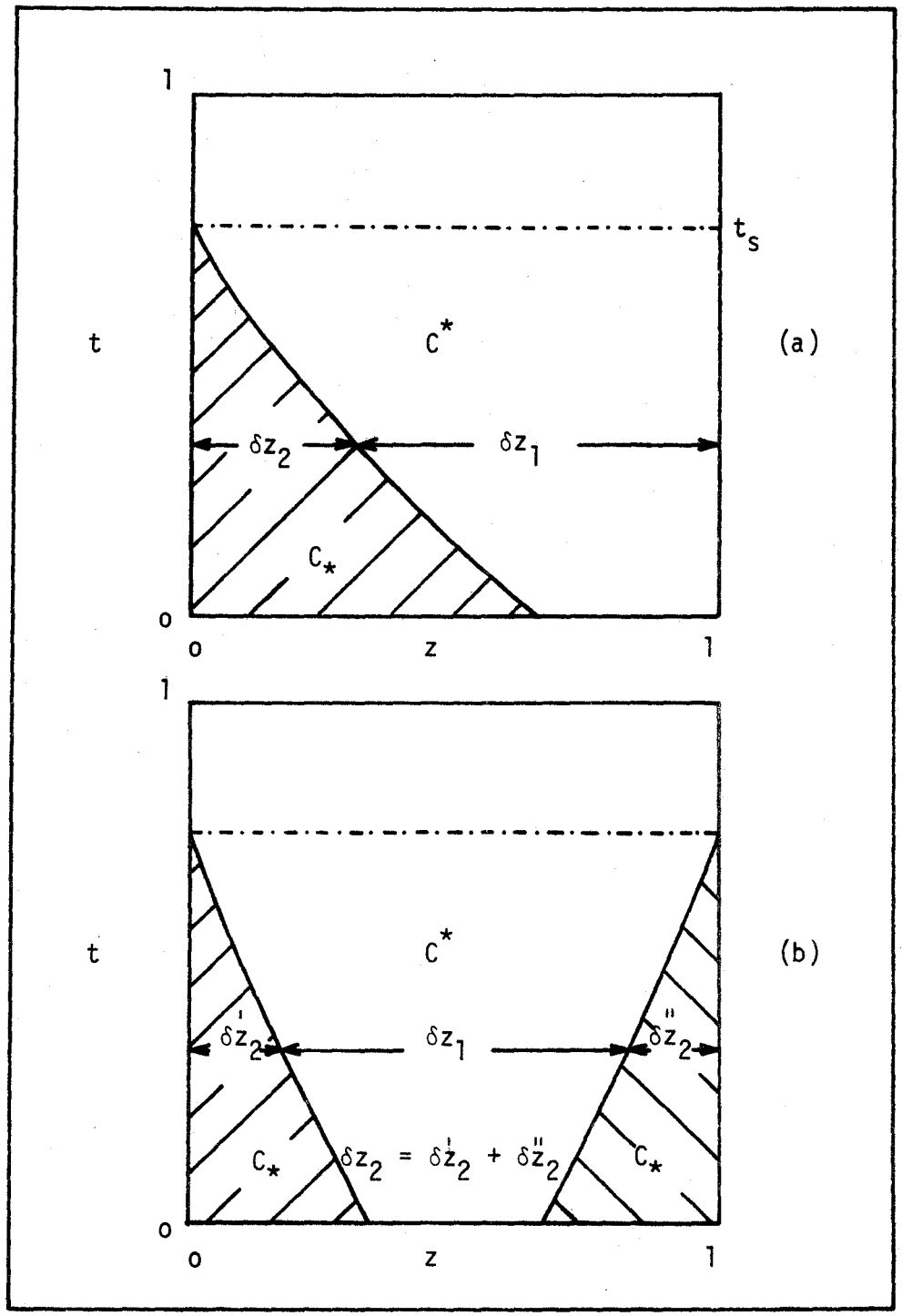

Figure 5-3 Equivalent Extremal Control Surfaces For A First-Order Catalyst Decay And $1 < p < \infty$.

Since, by assumption, the catalyst activity is independent of conversion in the reactor, then at any given time the catalyst activity and temperature at one point of the reactor have no influence on the catalyst activity and temperature at any other point of the reactor. This amounts to saying that at any given time interchanging parts of the bed with their respective activity and temperature does not change the exit conversion X(1,t) there.

Because of this, a single control switching line as in figure 5-3 (a) is considered in section 6 of that study concerned with the numerical evaluation of the extremal control policies.

5.5 p = 1

A special case of the optimal control problems is obtained when the kinetic parameter p = 1 since for that situation,

$$K(z,t) = A.k(z,t) \tag{5-180}$$

where the positive constant A is defined in (3-38), and the control k(z,t) appears only linearly in the state and costate equations (3-31), (3-32), (5-10) and (5-11). Defining:

$$\Gamma_1(z,t) = A.F_1(t).\psi(z,t) - \mu(z,t).g[\psi] \tag{5-181}$$

the function H given in (5-9) may be written accordingly,

$$H(z,t) = k(z,t).\Gamma_1(z,t) \tag{5-182}$$

where the function (5-181) is referred to in section 4.5 as the switching function. Clearly, the maximum of $H(z,t)$ corresponds to an extremal control $\hat{k}(z,t)$:

$$\hat{k}(z,t) = \begin{cases} k^* & \text{if } \Gamma_1(z,t) > 0 \\ \\ k_* & \text{if } \Gamma_1(z,t) < 0 \end{cases} \tag{5-183}$$

everywhere in τ where $\Gamma_1(z,t)$ has only isolated zeros.

Typical curves of the function H linear in the control k are illustrated in figure 5-4.

However, the possibility that the function (5-191) vanishes on non-empty open subsets $\delta\tau_1 \subseteq \tau$ may not be ruled out, that is,

$$\Gamma_1(z,t) = 0 \qquad \text{all } (z,t) \in \delta\tau_1 \subseteq \tau \tag{5-184}$$

and singular controls may exist in τ. A characteristic of such controls, discussed in section 4.5.1., is that,

$$\frac{\partial^q \Gamma_1(z,t)}{\partial t^q} = 0 \qquad q = 1, 2,... \tag{5-185}$$

and

$$\frac{\partial^{q'} \Gamma_1(z,t)}{\partial z^{q'}} = 0 \qquad q' = 1,2,... \tag{5-186}$$

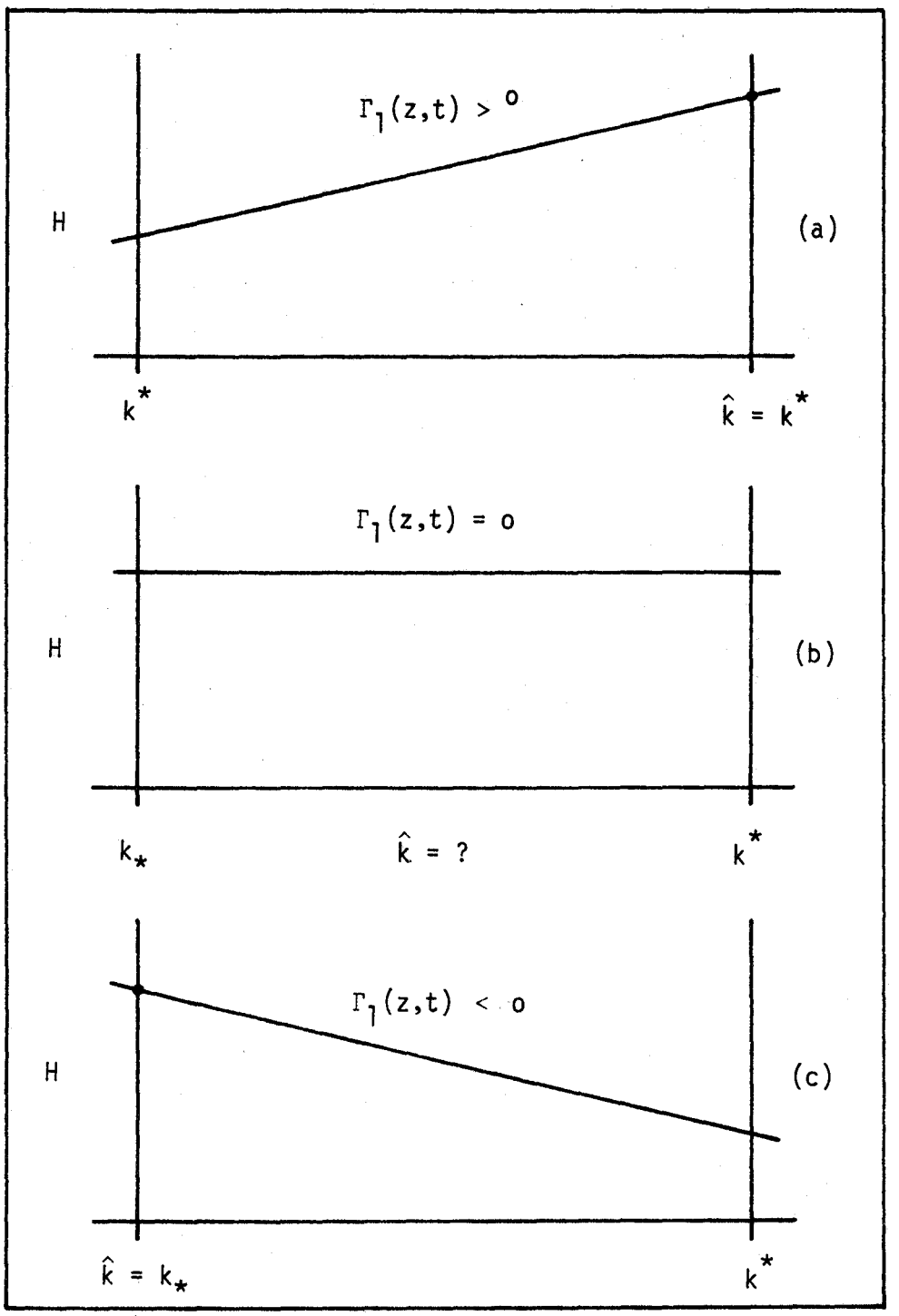

Figure 5-4 Typical Curves Of The Function H(z,t) Versus The Control $k_* \leqslant k(z,t) \leqslant k^*$ for p = 1.

in the interior of non-empty open subsets $\delta\tau_1 \subseteq \tau$.

The rate of change of the function $\Gamma_1(z,t)$ with time at any particular station of the reactor $z \in [0,1]$ may be written,

$$\frac{\partial \Gamma_1(z,t)}{\partial t} = \frac{\partial}{\partial t} \left\{ A.F_1(t).\psi(z,t) - \mu(z,t).g[\psi] \right\} \tag{5-187}$$

and using (3-32), (5-11) and (5-180),

$$\frac{\partial \Gamma_1(z,t)}{\partial t} = A.\psi(z,t).F_1'(t). \frac{dX(1,t)}{dt} \tag{5-188}$$

The case of a zero order reaction for which the rate (5-188) is zero is treated below and it is shown that an optimal control policy everywhere in τ may only be purely C^*.

Property 13:

When $\psi(z,t) > 0$ for all $z \in [0,1]$, then an optimal control policy for a zero order reaction may consist only of a pure policy C^* everywhere in τ, that is,

$$k^+(z,t) = k^* \qquad \text{all } (z,t) \in \tau$$

Proof:

Since at any time $t' \in [0,1]$, a zero order reaction is characterized by $F_1'(t) = 0$, equation (5-188) clearly indicates that,

$$\Gamma_1(z,t) = \text{constant} \tag{5-189}$$

everywhere in τ. Since at $t = 1$, $\mu(z,1) = 0$ and by equation (5-181)

$$\Gamma_1(z,1) > 0 \tag{5-190}$$

then because of (5-189), $\Gamma_1(z,t) > 0$ everywhere in τ and corresponding to optimality conditions (5-183),

$$\hat{k}(z,t) = k^* \qquad \text{all } z,t \in \tau \tag{5-191}$$

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When singular controls exists, then corresponding to each and every point $z,t \in \delta\tau_1$ where the condition $\psi(z,t).F_1'(t) \neq 0$ is validated, equation (5-188) with condition (5-185) and $q = 1$ give,

$$\frac{dX(1,t)}{dt} = 0 \tag{5-192}$$

thus indicating that the exit conversion $X(1,t)$ is a constant in time for all $z,t \in \delta\tau_1$.

Now since by properties 1 and 2, with the stated assumption,

$$\hat{k}(z,t) = k^* \tag{5-193}$$

for all $z \in [0,1]$ and $t \in (1-\delta t_o, 1]$, then to a non-increasing continuous inlet conversion $X_o(t)$ corresponds in time a decreasing continuous exit conversion $X(1,t)$, and,

$$\frac{dX(1,t)}{dt} < 0 \tag{5-194}$$

there.

Therefore, unless a reaction is zero order, $F_1'(t) < 0$ and (5-188) becomes,

$$\frac{\partial \Gamma_1(z,t)}{dt} > 0 \tag{5-195}$$

and since from (5-181) $\Gamma_1(z,1) > 0$ at $t = 1$, it would decrease from its positive value with decreasing time and could possibly attain a value zero for $t < 1$. When this occurs, the function $\Gamma_1(z,t)$ may become identically zero at one or many isolated stations $z_s \in [0,1]$ or uniformly zero along a finite length of the reactor $\Delta z \subseteq [0,1]$.

Since controls initiated at isolated stations $z_s \in [0,1]$ may satisfy the condition,

$$\Gamma_1(z_s,t) = 0 \tag{5-196}$$

for a finite interval of time, this case is investigated below.

Property 14:

> When the inlet conversion $X_o(t)$ is a non-increasing and continuous function of time $t \in [0,1]$ and if the function $\Gamma_1(z,t)$ becomes identically zero at times $t \in [0,1)$, for $\psi(z,t).F_1(t) > 0$, but only at isolated stations $z_s \in [0,1]$, then an extremal control policy in time may consist only of a bang-bang control policy at each and every station $z_s \in [0,1]$ with at most one switch in control from a policy C^* to a policy C_* in decreasing time.

Proof:

When at $t_s \in (0,1)$, but at isolated stations $z_s \in [0,1]$,

$$\Gamma_1(z_s,t_s) = 0 \qquad z_s \in [0,1] \tag{5-197}$$

with

$$\Gamma_1(z,t_s) > 0 \qquad z \in [0,1],\ z \neq z_s \tag{5-198}$$

a bang-bang switch in control may happen or a control satisfying condition (5-196) may be initiated at $t = t_s$ at stations $z_s \in [0,1]$, where,

$$t_s^- = \lim_{\substack{\delta t \to 0 \\ \delta t > 0}} \{t_s - \delta t\} \tag{5-199}$$

Assume first that a control satisfying condition (5-196), or

$$\frac{\partial \Gamma_1(z_s,t)}{\partial t} = 0 \tag{5-200}$$

is initiated at time t_s^- and exists for $0 \leqslant t < t_s$ at stations $z_s \in [0,1]$. Now since condition (5-200) and equation (5-188) indicate that,

$$\frac{dX(1,t)}{dt} = 0 \tag{5-201}$$

then result (5-201) with (5-188) make

$$\frac{\partial \Gamma(z,t)}{\partial t} = 0 \qquad t < t_s \tag{5-202}$$

for <u>all</u> $z \in [0,1]$, $z \neq z_s$, and the function $\Gamma_1(z,t)$ retains its posivity (5-198) for $t < t_s$. Therefore the control there is given by conditions (5-184) and,

$$\hat{k}(z,t) = k^* \qquad t < t_s,\ z \neq z_s \tag{5-203}$$

Recalling that the exit conversion $X(1,t)$ may be expressed as (see Appendix D),

$$X(1,t) = P[X_0(t), \int_0^1 k(\varepsilon,t).\psi(\varepsilon,t)d\varepsilon] \tag{5-204}$$

and that the contribution of the integral of the product $\{k(z_s,t).\psi(z_s,t)\}$,

$$\int_{z_s} k(\varepsilon,t).\psi(\varepsilon,t)d\varepsilon \tag{5-205}$$

over lengths of measure zero (isolated stations), to the integral of (5-204) is nil, then the exit conversion $X(1,t)$, corresponding to controls (5-203) and with a continuously and monotonically decreasing catalyst activity $\psi(z,t)$ in time and an inlet conversion $X_0(t)$ non-increasing in time, can only be a decreasing function of time. Therefore $X(1,t)$ cannot satisfy condition (5-201) and this violates assumption (5-200).

Consider now a switch in control actuated at $t = t_{\bar{s}}$,

$$\hat{k}(z_s,t) = k_* \qquad z_s \in [0,1] \tag{5-206}$$

Because of the arguments involved for integral (5-205) and the continuity of the catalyst activity and inlet conversion in time, at the limit for $t_{\bar{s}} \to t_s$:

$$X(1,t_{\bar{s}}) = X(1,t_s) \tag{5-207}$$

and

$$\left.\frac{dX(1,t)}{dt}\right|_{t = t_{\bar{s}}} < 0 \tag{5-208}$$

Therefore because of (5-208) condition (5-195) is recovered for $t = t_{\bar{s}}$, everywhere in Z^o, and $r_1(z,t)$ and $r_1(z_s,t)$ are then decreasing from their positive value (5-198) and zero value (5-197) respectively with decreasing time and,

$$r(z_s,t_{\bar{s}}) < 0 \tag{5-209}$$

with control (5-206) consistent with optimality conditions (5-183) there.

Since (5-208) is also true for $t < t_s$, it is then possible for $r_1(z,t)$ to become identically zero, backward in time, at other stations $z \in [o,1]$. If condition (5-197) is encountered at other times $t < t_s$ but only at isolated stations in Z^o for all $t \in (o,t_s)$, then the previous arguments hold and inequality (5-209) is always satisfied in this case with inequality (5-195) holding, everywhere in Z^o, for all $t \in [o,1]$.

Moreover, because of condition (5-195) holding throughout that time interval $\Delta t = [o,1]$ and everywhere in Z^o, a switch in control from a policy C^* to a policy C_* at these isolated stations may only occur once, backward in time.

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The case where the switching function $r_1(z,t)$ becomes identically zero in time but uniformly along a finite length of the reactor is also investigated and the results are summarized in the following.

Property 15:

> When the inlet conversion $X_o(t)$ is a non-increasing and continuous function of time $t \in [o,1]$ and if the function $\Gamma_1(z,t)$ becomes identically zero at times $t_s \in (o,1)$, for $\psi(z,t).F_1(t) > 0$, but uniformly along a finite length of the reactor $\Delta z \subseteq Z$, an extremal control policy in time cannot consist of a uniform jump in control over a finite length of the reactor $\delta z \subseteq \Delta z$ (bang-bang controls) at times $t_s \in (o,1)$. However singular control policies initiated at times $t_{\bar{s}}$ along stations $z \in \delta z$ may be extremal for $t < t_s$.

Proof:

Now when at $t_s \in (o,1)$,

$$\Gamma_1(\bar{z},t_s) = 0 \qquad \text{all } \bar{z} \in \Delta z \tag{5-210}$$

with

$$\Gamma_1(z,t_s) > 0 \qquad z \in [o,1],\ z \notin \Delta z \tag{5-211}$$

Assume first that a jump in control occurs at $t = t_{\bar{s}}$ uniformly along a finite length of the reactor $\delta z \subseteq \Delta z$, that is,

$$\hat{k}(\hat{z},t_{\bar{s}}) = k_* \qquad \text{all } \hat{z} \in \delta z \tag{5-212}$$

with controls (5-193) existing at all other stations for $t = t_{\bar{s}}$, defined in (5-199).

The exit conversion may then be expressed at time $t = t_s$ by,

$$X(1,t) = P[X_o(t_s), \int_o^1 k^*.\psi(\varepsilon,t_s).\, d\,\varepsilon] \tag{5-213}$$

and at time $t = t_{\bar{s}}$ by,

$$X(1,t_{\bar{s}}) = P[X_o(t_{\bar{s}}), \int_{\delta z} (k_*-k^*).\psi(\varepsilon,t_{\bar{s}}).\, d\,\varepsilon + \int_o^1 k^*.\psi(\varepsilon,t_{\bar{s}})\, d\,\varepsilon\,] \tag{5-214}$$

Because of the continuity of $X_o(t)$ and $\psi(z,t)$ in time and the fact that the integral of the product $\{(k_*-k^*).\psi(z,t_{\bar{s}})\}$ over a finite length δz is negative, at the limit for $t_{\bar{s}} \to t_s$,

$$X(1,t_{\bar{s}}) < X(1,t_s) \tag{5-215}$$

and for a non-zero order reaction,

$$F_1(t_{\bar{s}}) > F_1(t_s) \tag{5-216}$$

then from (5-181) since $\mu(z,t)$ is a continuous function of time (see Appendix D),

$$\Gamma_1(\delta,t_{\bar{s}}) > \Gamma_1(\delta,t_s) \qquad \text{all } \delta \in [o,1] \tag{5-217}$$

However from (5-210) and (5-211) and inequality (5-217), the switching function for $t = t_{\bar{s}}$ is positive everywhere in Z^o and in accord with optimality conditions (5-186),

$$k(\delta,t_{\bar{s}}) = k^* \qquad \text{all } \delta \in [o,1] \tag{5-218}$$

Result (5-218) then contradicts assumption (5-212) and a jump in control initiated at $t = t_{\bar{s}}$ uniformly along some finite length of the reactor $\delta z \subseteq \Delta z$ is not optimal.

Now consider controls initiated at $t = t_{\bar{s}}$ along a finite length of the reactor $\delta z \subseteq \Delta z$ such that for $t < t_s$,

$$\frac{\partial r_1(\hat{z},t)}{\partial t} = 0 \qquad \hat{z} \in \delta z \qquad (5\text{-}219)$$

Condition (5-219) with (5-188) indicates however that

$$\frac{dX(1,t)}{dt} = 0 \qquad t < t_s \qquad (5\text{-}220)$$

and consideration of (5-220) with (5-188) at other stations $z \in [0,1]$ show that,

$$\frac{\partial r_1(\delta,t)}{\partial t} = 0 \qquad \text{all } \delta \in [0,1] \qquad (5\text{-}221)$$

and the function $r_1(z,t)$ retains its posivity (5-211) and $r_1(\bar{z},t)$ remains zero (5-210) for $t < t_s$ where (5-219) holds. Controls at these stations for $t = t_{\bar{s}}$ are then given according to conditions (5-183) at stations $z \in [0,1]$, $z \notin \Delta z$, and

$$\hat{k}(z,t_{\bar{s}}) = k^* \qquad (5\text{-}222)$$

but for all $\bar{z} \in \Delta z$,

$$\hat{k}(\bar{z},t_{\bar{s}}) = \bar{k}(\bar{z},t_{\bar{s}}) \qquad (5\text{-}223)$$

where $\bar{k}(\bar{z},t_{\bar{s}})$ is an admissible singular control $\in [k_*,k^*]$. Condition (5-220) implied by (5-219) then requires by relation (5-215) that the control $\hat{k}(\bar{z},t)$

be chosen in time for all $\bar{z} \in \Delta z$ such that,

$$X(1,t) = \text{constant} \tag{5-224}$$

for $t < t_s$, where

$$X(1,t) = P[X_o(t), \int_{\Delta z} \hat{k}(\varepsilon,t).\psi(\varepsilon,t).d\,\varepsilon + \int_{Z^o \setminus \Delta z} k^*.\psi(\varepsilon,t).d\,\varepsilon] \tag{5-225}$$

Because the catalyst activity is a continuous and monotonic decreasing function of time and the inlet conversion $X_o(t)$ is also a continuous and non-increasing function of time, controls $\hat{k}(\bar{z},t)$, $\bar{z} \in \Delta z$, may then be decreased backward in time, from their maximum value k^* at $t = t_s$, in order to satisfy (5-224).

When ultimately $\hat{k}(\bar{z},t)$ reaches the lower limit k_* everywhere in Δz before $t = 0$ is attained, say $t = t_c$, then for $t = t_c^-$ condition (5-224) may no longer be satisfied, and,

$$\frac{dX(1,t)}{dt} < 0 \qquad t = t_c^- \tag{5-226}$$

with t_c^- having the same significance as in (5-199).

Because of (5-226) condition (5-195) is recovered everywhere in Z^o for $t = t_c^-$ and then the function $r_1(z,t)$ will decrease from its positive value (5-210) and $r_1(\bar{z},t)$ from its zero value, with decreasing time, and,

$$r_1(\bar{z},t_c^-) < 0 \tag{5-227}$$

with the corresponding control $\hat{k}(\bar{z},t_c^-) = k_*$ in accord with conditions (5-183). Since it is possible for $r_1(z,t)$, $z \in [o,1]$, $z \notin \Delta z$, to reach a value zero uniformly along another finite segment of the reactor for $t < t_c$, the previous

arguments remain valid there and either condition (5-195) or (5-221) will always be satisfied in this process for all $t \in [o,1]$.

Hence by condition (5-195) once a singular control has reached the lower constraint k_* backward in time, and the switching function becomes negative there, it stays there until $t = 0$.

★

It is shown in property 15 that an extremal control policy in time at any station $z \in [o,1]$, may consist only of one of the following policies,

Type I	policy $\{C^*\}$	all $t \in [o,1]$
Type IV	policy $\begin{Bmatrix} Sg \\ C^* \end{Bmatrix}$	$0 \leqslant t \leqslant t^*$ $t^* \leqslant t \leqslant 1$
Type V	policy $\begin{Bmatrix} C_* \\ Sg \\ C^* \end{Bmatrix}$	$0 \leqslant t \leqslant t_*$ $t_* \leqslant t \leqslant t^*$ $t^* \leqslant t \leqslant 1$

where Sg refers to a singular control policy.

Property 16:

> When the inlet conversion $X_o(t)$ is a non-increasing function of time and when the function $r_1(z,t)$, corresponding to a first-order catalyst deactivation process, becomes identically zero in time, it then becomes uniformly zero along the entire reactor bed independently of the catalyst activity profile there.

Proof:

For a first-order deactivation process $g[\psi] = \psi$ and equation (5-11) may be written using (5-5) and (D-18),

$$\frac{\partial \mu(z,t)}{\partial t} = \{\mu(z,t) - A.F_1(t)\} .k(z,t) \qquad (5\text{-}228)$$

with the terminal condition $\mu(z,1) = 0$ everywhere in Z^o at $t = 1$. Recalling properties 1 and 2, with the given assumptions, control (5-193) exists everywhere in Z^o for time $t \in (1-\Delta t, 1]$, with $\Delta t > 0$, and considering (5-228) the variable $\mu(z,t)$ has a uniform value everywhere in Z^o for times $t \in (1-\Delta t, 1]$. When at time $t = 1-\Delta t$, the switching function $\Gamma_1(z,t)$ becomes identically zero at one station $z \in [o,1]$,

$$\Gamma_1(z,t) = \psi(z,t). \{A.F_1(t) - \mu(z,t)\} \qquad (5\text{-}229)$$

clearly since the only position dependent variable $\mu(z,t)$ inside the parenthesis of (5-229) is uniform in value everywhere in Z^o at that time and $\psi(z,t) > 0$ by assumption, then the parenthesis of (5-229) is uniformly zero in value for all $z \in [o,1]$ independently of the catalyst activity profile $\psi(z,t)$ there.

★

Therefore extremal control policies pertaining to such catalyst decay process may only be of type I, IV or V.

CHAPTER 6

NUMERICAL EVALUATION OF EXTREMAL POLICIES AND DISCUSSION

6.1. Hypothetical Reactor

In order to illustrate the various control policies, numerical calculations of extremal policies are carried out for the following hypothetical reactor,

$$\frac{\partial X}{\partial z} = K[T].F[X].\psi \tag{6-1}$$

and

$$\frac{\partial \psi}{\partial t} = - k[T].g[\psi] \tag{6-2}$$

for $F[X] = [1-X]^n$ and $g[\psi] = \psi^m$. Both functions K[T] and k[T] are assumed of the Arrhenius form and are defined respectively by (3-28) with (3-10) and (3-29) with (3-21).

The inlet conversion to the reactor $X_o(t)$ is considered a constant,

$$X_o(t) = o. \qquad \text{all } t \in [0,1] \tag{6-3}$$

for all numerical cases studied, but the initial catalyst activity profile in the reactor is assumed to have the following piecewise continuous distributions,

$$\text{i} \quad - \psi_o(z) = C_1 \qquad \text{all } z \in [0,1] \tag{6-4}$$

$$\text{ii} - \psi_o(z) = C_2.\exp\{C_3.(1-z)\} \qquad \text{all } z \in [0,1] \tag{6-5}$$

$$\text{iii} - \psi_0(z) = C_4 \qquad z \in [0, z_1]$$

$$\psi_0(z) = C_5 \qquad z \in [z_1, 1] \tag{6-6}$$

with C_i, $i = 1,\ldots,5$ representing constants.

Numerical values of $n = 0.5$, 1.0 and 2.0 and $m = 0.75, 1.0$ and 2.0 are considered for the reaction and deactivation orders respectively. The reactor average space time is,

$$t_\Theta = 1 \text{ sec.} \tag{6-7}$$

and the total operational time,

$$t_f = 2.16 \times 10^6 \text{ sec. (25 days)} \tag{6-8}$$

Upper and lower bounds placed on the admissible temperature are,

$$T^* = 900.^\circ K$$

$$T_* = 700.^\circ K \tag{6-9}$$

The catalyst deactivation energy,

$$E_c/R = 15{,}000.^\circ K \tag{6-10}$$

with a rate constant for deactivation,

$$k_0^{\dagger} = 20.2447 \text{ (1./sec.)} \qquad (6\text{-}11)$$

as defined in (3-15) are considered. For a given value of the parameter p, the reaction activation energy E_R/R is easily calculated from (3-39). The reaction rate constant K_0 of K[T] is computed using equations (6-1), with condition (6-3) for all reaction orders, corresponding to a maximum attainable exit conversion $X_1^*(1,t) = 0.90$ with fresh catalyst $\psi(z,t) = 1.0$ and maximum temperature $T^* = 900.^{o}K.$ everywhere in the reactor. Reaction activation energies E_R/R and reaction rate constants K_0 are listed in table 6-1 corresponding to sets of parameters n and p describing cases further investigated below.

6.2. Algorithmic Procedure

Since the quality of extremal controls in time differs markedly for values of p larger or smaller than unity, the structure of the synthesizing algorithms likewise differs for values of $p > 1$ or $p < 1$ and two basic extremal control synthesizing algorithms have been constructed to solve each case separately.

No algorithm has been specifically constructed for the physically possible, but unlikely, case of $p = 1.0$ exactly. The solution to this problem may be found at the limit for $p \to 1$ with values of p above or below but arbitrarily close to unity from the appropriate basic algorithm.

The consideration of a first-order catalyst deactivation process always led to the identification of additional properties of the extremal control policies and these are used with profit in devising a simpler and/or more efficient version for each of the basic algorithms.

† The large number of significant figures retained is due to back calculation using $k[T_*] = 10^{-8}$(1./sec.).

p	n	K_o	E_R/R
		(1/sec)	$^oK.$
0.10	1.0	1.21910×10^{1}	1500.
0.50	0.5	5.68934×10^{3}	7500.
0.50	1.0	9.57936×10^{3}	7500.
0.50	2.0	3.74424×10^{4}	7500.
0.90	1.0	7.52719×10^{6}	13500.
1.10	1.0	2.10999×10^{8}	16500.
1.50	0.5	9.84699×10^{10}	22500.
1.50	1.0	1.65797×10^{11}	22500.
1.50	2.0	6.48044×10^{11}	22500.
2.50	1.0	2.86959×10^{18}	37500.
5.0	1.0	3.57621×10^{36}	75000.

Table 6-1. Reaction Activation Energy E_R/R And Rate Constant K_o Corresponding To A Reaction Order n And Kinetic Parameter p.

In summary, the following algorithms have been constructed:

Basic algorithm	C1 : $p > 1, m \neq 1$
" "	S1 : $p < 1, m \neq 1$
Sub-algorithm	C2 : $p > 1, m = 1$
" "	S2 : $p < 1, m = 1$

All of these algorithms are iterative in nature in the sense that,

1. a control surface $\hat{k}(z,t)$ defined in τ, obeying some but not necessarily all of the properties of an extremal control surface, is assumed,
2. the state and costate equations are solved using that control surface and the given initial, terminal and boundary conditions,
3. the maximum condition (4-16) is used with these pseudo-extremal state and costate variables to generate a pseudo-extremal control surface $\hat{k}(z,t)$,
4. this pseudo-extremal control surface is assumed to be the extremal one and step 2. to 3. are repeated. When, after a finite number of iterations no significant change between the assumed and generated control surface is found and when the maximum condition is everywhere satisfied, then this control surface is an extremal one.

Although no quarantee of convergence is given for such iterative process, convergence was achieved in all cases surveyed.

All of these algorithms use the method of characteristics which is probably the best technique for solving the state and costate equations. For the quasi-steady state problem considered here the characteristic lines are parallel to the t and z axes, making the technique very simple.

These characteristic lines are illustrated in figure 6-1. Denoting by I_ℓ the t = constant characteristic line, and by II_ℓ the z = constant characteristic line, then equations (3-31) and (3-32) become ordinary differential equations along I_ℓ and II_ℓ respectively.

A brief description of the basic steps characterizing each of these different algorithms is given below.

6.2.1. Algorithm C1 : $p > 1, m \neq 1$

Step 1. Because of property 9, assume a control switching line separating the plane of τ in two distinct regions where controls k^* and k_* are defined. By properties 1 and 2 this control switching line must not be touching the line t = 1 and because of property 11, it must not contain any segment parallel to the z axis.

Step 2. With initial condition (3-35), integrate equation (3-32) in time from $0 \leqslant t \leqslant 1$ along lines II_i, i = 0,...,M with the control defined in step 1., and store the value $\psi(z_i,t_j)$ at all mesh points.

Step 3. With boundary condition (3-33), integrate equation (3-31) along the reactor for $0 \leqslant z \leqslant 1$ along line I_j, j = 0,...,N with the control defined in step 1. and $\psi(z_i,t_j)$ computed in step 2. Store the values of $X(1,t_j)$, j = 0, ...,N.

Step 4. For each line II_i, i = 0,...,M starting backward in time from t = 1 where by properties 1 and 2 ΔK and Δk are defined by (5-108) and (5-109), locate the time at which $\Delta H(z_i,t_j)$ computed by (5-107) first becomes negative and then by interpolation the precise time at which it first becomes zero. Label these times t_{si}, i = 0,...,M and store.

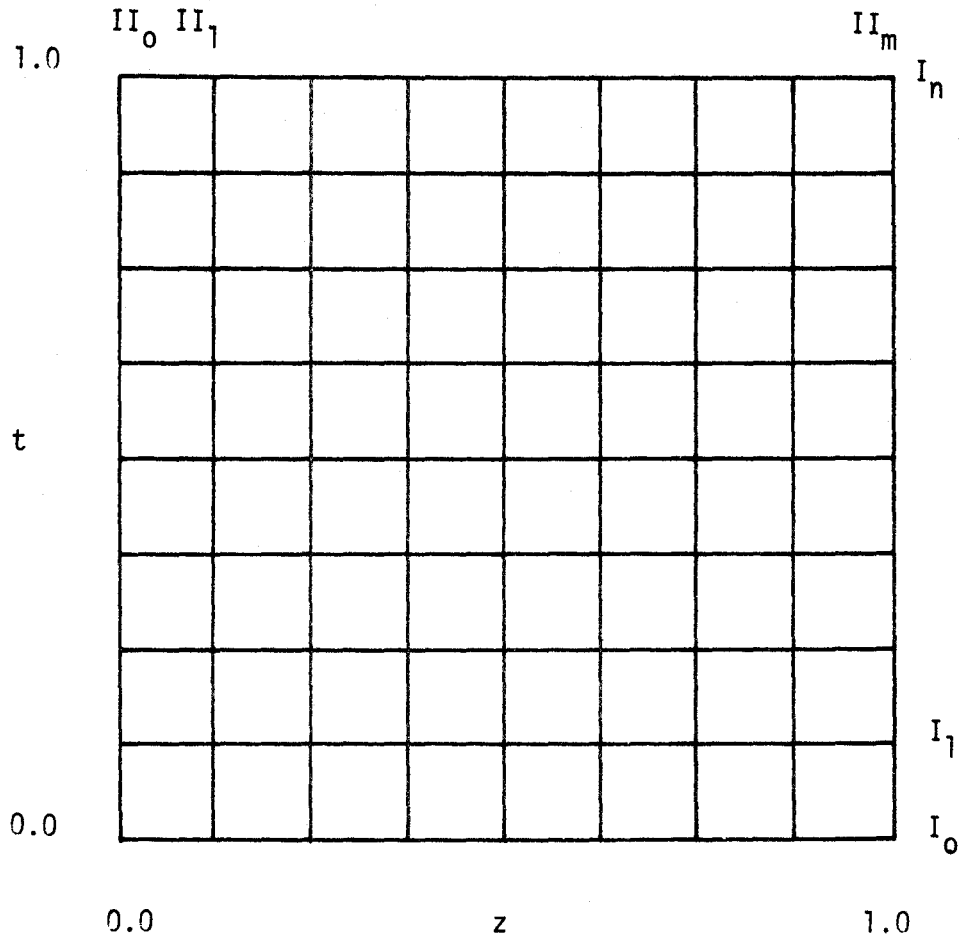

Figure 6-1 Characteristic Lines For The State And Costate Variables In The Plane Of Z^o x T^o.

Step 5. Determine if the line joining these points (z_i, t_{si}), $i = 1,\ldots,M$, differ significantly according to some defined measure, such as,

$$E_1 = \sum_{i=0}^{M} [t_{si_{new}} - t_{si_{old}}]^2 \qquad (6\text{-}12)$$

from the previous assumed control switching line.

If so then take this newly generated line as the new control switching line and go to step 2. If not then proceed to step 6.

Step 6. At each and every mesh point defined by lines I_j and II_i compute $\Delta H(z_i, t_j)$ according to (5-107) using ΔK and Δk given by (5-108) and (5-109) for $t \geq t_{si}$ and $(-\Delta K)$ and $(-\Delta k)$ for $t < t_{si}$. If $\Delta H(z_i, t_j) \geq 0$ everywhere at these mesh points then this control switching line is an extremal one with respect to the set of mesh points $\varepsilon\ \tau$.

Although this condition was satisfied for all the cases surveyed, if it were to be violated at one or more mesh points this would indicate that a single control switching line is not sufficient to describe an extremal control surface defined in τ. The same basic procedure discussed here could then be extended to two or more extremal control switching line candidates starting with step 1.

A typical rate of convergence of this algorithm with respect to the number of iterations is illustrated in figure 6-2.

6.2.2. Algorithm C2 : p > 1, m = 1

Step 1. Set $\ell = 1$.

Step 2. Choose at time $t_o = 0$. a station $z_{so}^{\ell} \varepsilon (0,1)$ which divides the reactor in two sections δz_1 and δz_2 with their respective control k^* and k_*. Compute

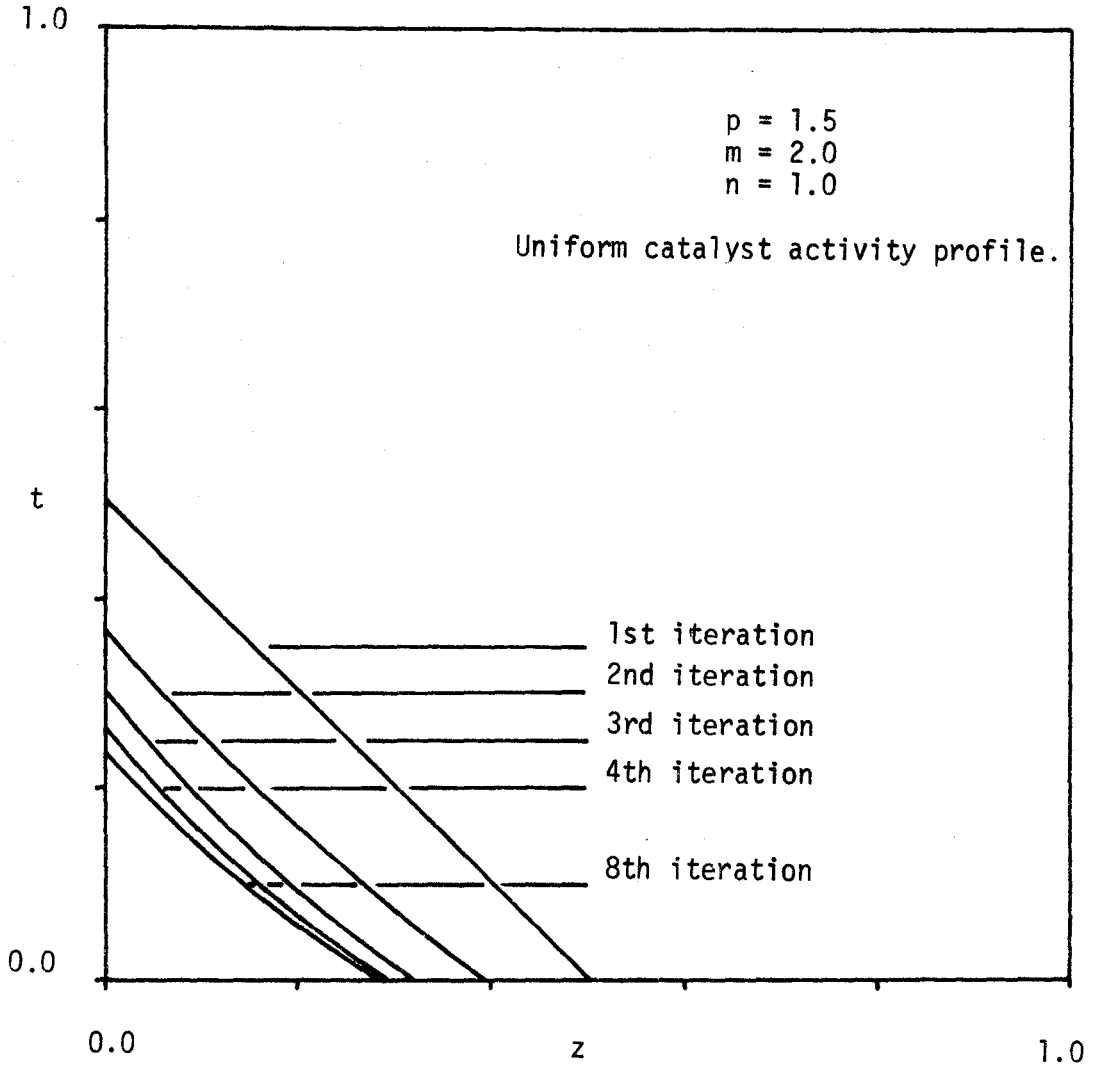

Figure 6-2 Typical Rate Of Convergence Of A Control Switching Line In The Plane Of Z^o x T^o For Algorithm C1.

the conversion $X(1,t_o)$ using equations (D-5) or (D-6) with the boundary condition (3-33) and initial catalyst activity profile (3-35).

Step 3. Set $j = 1$.

Step 4. Now for $t = t_j$ find a station $z^{\ell}_{sj} \in [0,1]$ such that by joining the points $(z^{\ell}_{s_{j-1}}, t_{j-1})$, (z^{ℓ}_{sj}, t_j) a segment of a control switching line is constructed such that the resulting conversion $X(1,t_j)$, obtained by using (D-5) or (D-6) with (D-11) and the initial and boundary conditions (3-35) and (3-33), has the value predicted by equation (5-177).

Step 5. Repeat step 4. for other times t_j, $j = 2, 3,...$ and locate the time t^{ℓ}_c at which the control switching line thus defined intercepts the line $z = 0$. Store t^{ℓ}_c.

Step 6. With initial condition (3-35) and equation (D-11), compute $\psi(z_i,t_j)$ in time for $0 \leqslant t \leqslant 1$ along lines II_i, $i = 0,...,M$ and t_j, $j = 0,...,N$ with the control defined in step 4. Store the values of $\psi(z_i,t_j)$ at all mesh points.

Step 7. With boundary conditions (3-33) and equation (D-5) or (D-6), compute $X(z,t)$ along the reactor length for $0 \leqslant z \leqslant 1$ along line I_j, $j = 0,...,N$ with the control defined in step 4. and $\psi(z_i,t_j)$ given in step 6. Store the values of $X(1,t_j)$ for $j = 0,...,N$.

Step 8. Since for a first-order catalyst deactivation process when $\Delta H(z,t)$ first reaches a value zero backward in time from the line $t = 1$, it reaches it uniformly along the whole reactor bed, locate the time at which $\Delta H(z,t)$ computed by (5-107) first become zero at any chosen station $z \in [o,1]$. Label this time t^{ℓ}_H and store.

Step 9. Form an error function,

$$E^{\ell}_2 = [t^{\ell}_H - t^{\ell}_c]^2 \qquad (6\text{-}13)$$

corresponding to the guess Z_{so}^{ℓ} done in step 2, and t_c^{ℓ} and t_H^{ℓ} are found in step 5. and 8.

Step 10. Repeat step 2. with $\ell = 2, 3, \ldots$ using a new guess Z_{so}^{ℓ} each time and following steps 3. to 9. find a station $\hat{Z}_{so}^{\ell}$ such that the function (6-13) is minimized. When E_2^{ℓ} is minimized with $E_2^{\ell} \to 0$ at the limit for a finite number ℓ, the control switching line generated in step 4. and for which the maximum condition $\Delta H(z,t) \geq 0$ is satisfied everywhere in τ is an extremal one.

A typical rate of convergence of algorithm C2 with respect to the number of iterations is illustrated in figure 6-3.

6.2.3. Algorithm S1 : $p < 1$, $m \neq 1$

Step 1. Corresponding to the intersections of the line $t = 0$ with each line II_i, $i = 0,\ldots,M$ assume a control $k(z_i, 0)$ such that,

$$k_* < k(z_i, 0) < k^* \tag{6-14}$$

and store.

Step 2. With boundary conditions (3-33) and equation (D-5) or (D-6) compute $X(1,0)$ using the initial catalyst activity profile (3-35) and the controls defined in step 1. Store $X(1,0)$.

Step 3. Considering $X_0(t)$ = constant, then for times where the whole bed is on a stationary policy S, sub-property 6[a] indicates that $X(1,t)$ = constant. Therefore for each line II_i, $i = 0,\ldots,M$ assuming the whole bed is on a stationary policy S in time the activity $\psi(z_i, t_i^*)$, where $t_i^* \in (0,1]$ refers to the time at which $k(z_i, t_i^*) = k^*$, may be computed with relation (5-63) using controls

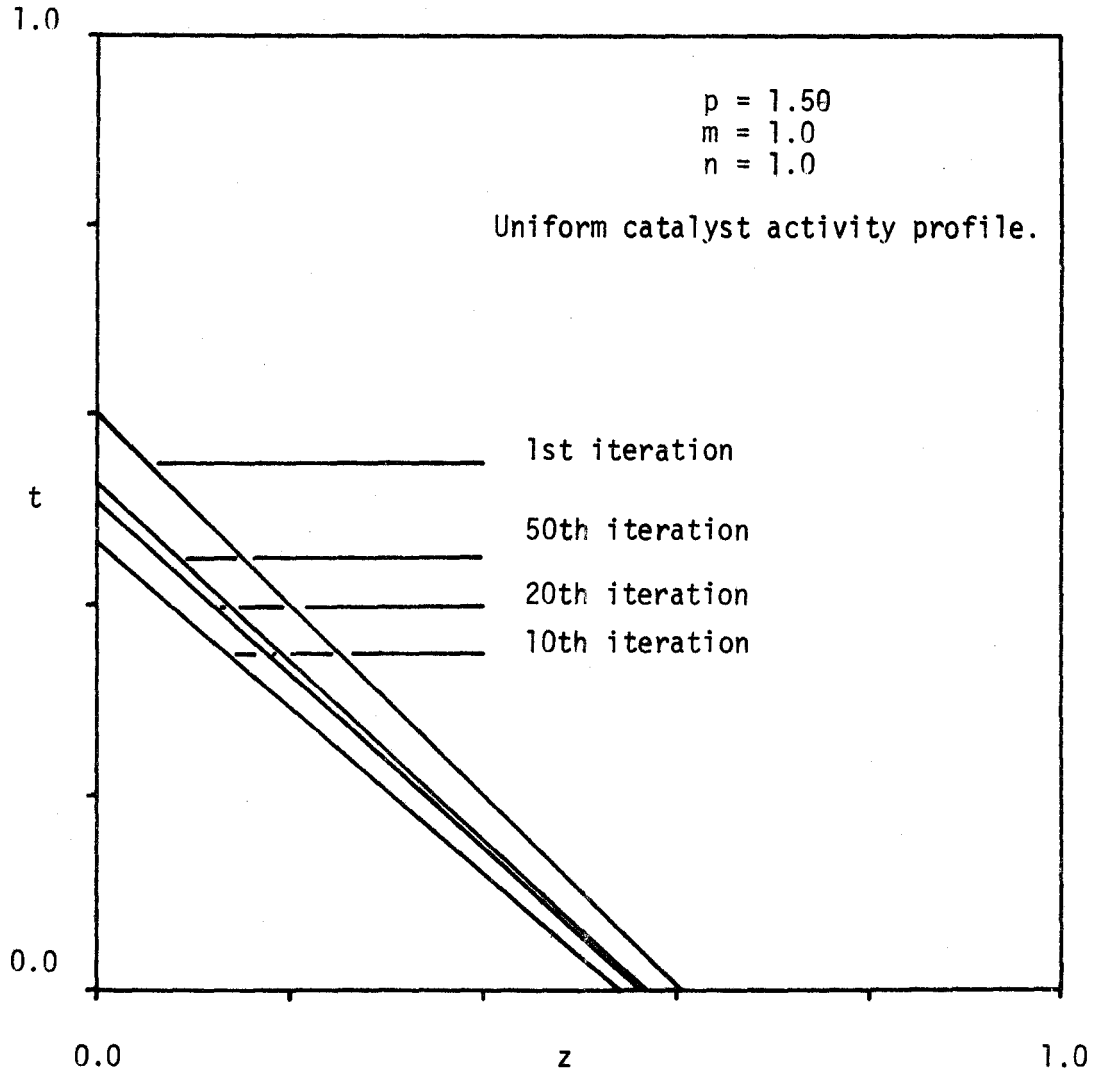

Figure 6-3 Typical Rate Of Convergence Of A Control Switching Line In The Plane Of Z^{O} x T^{O} For Algorithm C2.

from step 1. and X(1,0) from step 2. and the initial condition (3-35). Store $\psi(z_i,t_i^*)$, i = 0,...,M.

Step 4. Using relation (5-63) the control $k(z_i,t)$ on a stationary policy S may be conveniently expressed as a function of $\psi(z_i,t)$ and of the known quantities $\psi(z_i,0)$, $k(z_i,0)$ and X(1,t) = X(1,0) = constant. Substituting this expression in equation (3-32) and integrating from time t = 0 to $t = t_i^*$, the values of t_i^*, i = 0,...,M may be calculated since corresponding to each line II_i both values of $\psi(z_i,0)$ and $\psi(z_i,t_i^*)$ are known from (3-35) and step 3. Store t_i^*, i = 0,...,M.

Step 5. Find the upper and lower bounds from the set t_i^*, i = 0,...,M and label t_{max} and t_{min} respectively. Now for $t \leqslant t_{min}$ the whole bed is on a stationary policy S and the assumption of constant exit conversion is validated for $t \in [0,t_{min}]$. If $t_{max} = t_{min}$ go to step 12 otherwise proceed to step 6.

Step 6. For time $t \in \Delta t = [t_{max} - t_{min}]$ the whole bed is not on a S policy and X(1,t) ≠ constant. Compute the value of $\psi(z_i,t_{min})$ using equation (3-32) upon substitution of (5-63) for k and integrate from t = 0 to $t = t_{min}$. Use relation (5-63) and compute $k(z_i,t_{min})$. Store both $\psi(z_i,t_{min})$ and $k(z_i,t_{min})$ for i = 0,...,M.

Step 7. Compute corresponding to each line II_i, i = 0,...,M the values of $\psi(z_i,t)$ for time $t \in [t_i^* - t_{min}]$ using equation (3-32) substituted for k with (5-63) and integrating from $t = t_{min}$ to t = t using boundary condition $\psi(z_i,t_{min})$ known from step 6. Then compute for each of these times $t \in [t_i^* - t_{min}]$ the corresponding control $k(z_i,t)$ using (5-63). Store all computed values.

Step 8. Integrating along lines parallel to the axis of the reactor, compute X(1,t) using equation (D-5) or (D-6) with condition (3-33) and activity $\psi(z_i,t)$ and control $k(z_i,t)$ defined in step 7.

Step 9. Using this new conversion profile $X(1,t)$ as the current one, compute for each line II_i, $i = 0,\ldots,M$ with the results $\psi(z_i,t_{min})$ and $k(z_i,t_{min})$ of step 6. the new values of $\psi(z_i,t_i^*)$. Store all values $\psi(z_i,t_i^*)$, $i = 0,\ldots,M$.

Step 10. Using relation (5-63) the control $k(z_i,t)$ on a stationary policy S may be conveniently expressed as a function of $\psi(z_i,t)$ and of the known quantities $\psi(z_i,t_{min})$, $k(z_i,t_{min})$ and current $X(1,t)$. Substituting this expression in equation (3-32) and integrating from time $t = t_{min}$ to $t = t_i^*$, the values of t_i^*, $i = 0,\ldots,M$ may be calculated since corresponding to each line II_i both values of $\psi(z_i,t_{min})$ and $\psi(z_i,t_i^*)$ are known from step 6. and 9. Store all values of new t_i^*, $i = 0,\ldots,M$.

Step 11. Find the new upper bound from the set of t_i^*, $i = 0,\ldots,M$ newly defined, t_{min} remaining the same value, and repeat steps 7. through 10. until according to some measure,

$$E_3 = \sum_{i=0}^{M} [t_{i_{old}}^* - t_{i_{new}}^*]^2 \qquad (6\text{-}15)$$

E_3 is minimized with $E_3 \to 0$. Then store all values of the current iteration and proceed to step 12.

Step 12. With condition $\psi(z_i,t_i^*)$ and equation (D-12) compute along each line II_i, $i = 0,\ldots,M$ the value of $\psi(z_i,t)$ for time $t_i^* \leqslant t \leqslant 1$ using control $k = k^*$. Store all computed values.

Step 13. With boundary condition (3-33) and equation (D-5) and (D-6) compute $X(1,t)$ for $t \varepsilon \Delta t = (1\text{-}t_{max})$ using results of step 12. and control $k = k^*$. Store $X(1,t)$.

Step 14. For each line II_i, $i = 0,\ldots,M$ locate starting from $t = 1$, backward in time, the time at which $\frac{\partial H}{\partial k}$ first becomes zero. $\frac{\partial H}{\partial k}$ is computed by equation

(5-25) with relation (D-25) using (D-12) with everywhere a control $k = k^*$ and where the boundary and terminal conditions $X(1,t)$ and $\psi(z,1)$ are given in step 12. and 13. Label these times t_i^o, $i = 0,\ldots,M$ and store.

Step 15. Defining a new time,

$$t_i^+ = (t_i^* + t_i^o)/2 \tag{6-16}$$

at which $k(z_i,t_i^+) = k^*$, compute using $k = k^*$ for $t \in \Delta t = (1-t_i^+)$ the value of $\psi(z_i,t_i^+)$ using (D-12) with the terminal condition $\psi(z_i,1)$ computed in step 12. Store all values of t_i^+, $i = 0,\ldots,M$.

Step 16. A new initial control $k(z_i,0)$ may then be calculated by using relation (5-63) with the current $X(1,t)$ profile available and initial condition (3-35) plus the results $k(z_i,t_i^+) = k^*$ and $\psi(z_i,t_i^+)$ given in step 15.

Step 17. Steps 1. through 16. may then be repeated until the measure,

$$E_4 = \sum_{i=0}^{M} \{[k(z_i,0)_{old} - k(z_i,0)_{new}]^2 + [t_i^* - t_i^o]^2\} \tag{6-17}$$

is minimized with $E_4 \to 0$. Then the control surface $k(z,t)$ for all $(z,t) \in \tau$ satisfying everywhere the maximum condition is an extremal one.

A typical rate of convergence of this algorithm with respect to the number of iterations is illustrated in figure 6-4.

6.2.4. Algorithm S2 : $p < 1$, $m = 1$

For a first-order catalyst deactivation process properties 8 and 8a hold and an extremal control is uniform for all $z \in [0,1]$ at any given time $t \in [0,1]$.

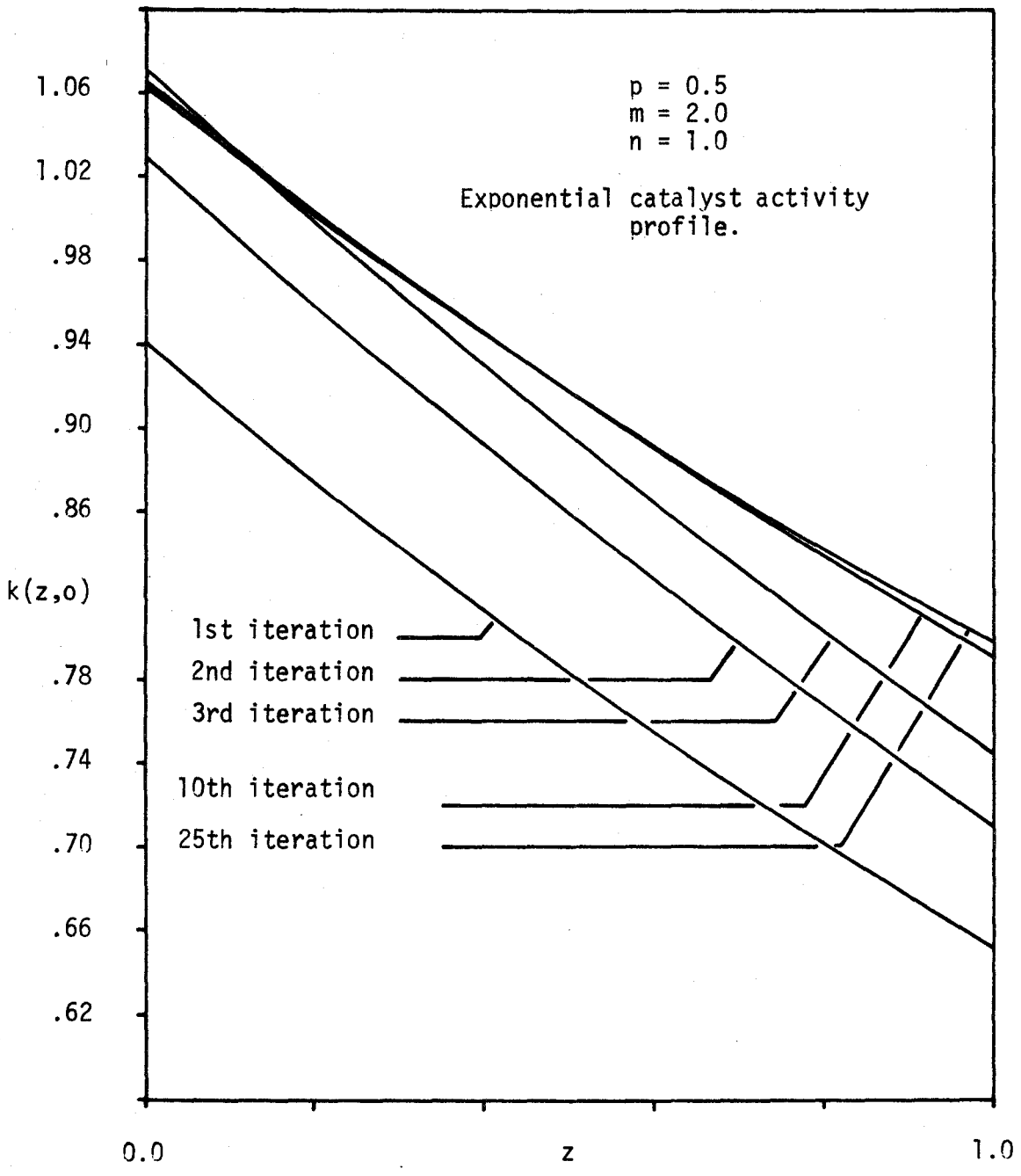

Figure 6-4 Typical Rate Of Convergence Of The Initial Control k(z,o) Along The z Axis For Algorithm S1.

Therefore algorithm S2 uses the same basic steps of algorithm S1 but with the following modifications:

Step 1. Assume a uniform control value such that at time t = 0,

$$k_* < k_0(t) < k^* \tag{6-18}$$

Step 4. Same, except that by sub-property 8a only one value of $t_i^* = t^*$ need be calculated.

Step 5. Go to step 12. with $t_{min} = t_{max} = t^*$.

Step 14. Same, except that by property 8 only one time $t_i^o = t^o$ need be located and stored.

Step 15. Same with a single $t_i^+ = t^+$ defined.

Step 16. Same but with a single control $k_0(0)$.

Step 17. Same but with,

$$E_4 = [k_0(0)_{old} - k_0(0)_{new}]^2 + [t^* - t^o]^2 \tag{6-19}$$

Figure 6-5 illustrates a typical rate of convergence of this algorithm with respect to the number of iterations T_0 representing the uniform starting temperature, T(z,0) all $z \in [0,1]$.

6.3. Effect Of Kinetic Parameters On Extremal Policies

6.3.1. Reaction Order n

Recalling from property 10 that for $p > 1$ an optimal control policy for a zero-order reaction is purely k^* everywhere in τ, an optimal control

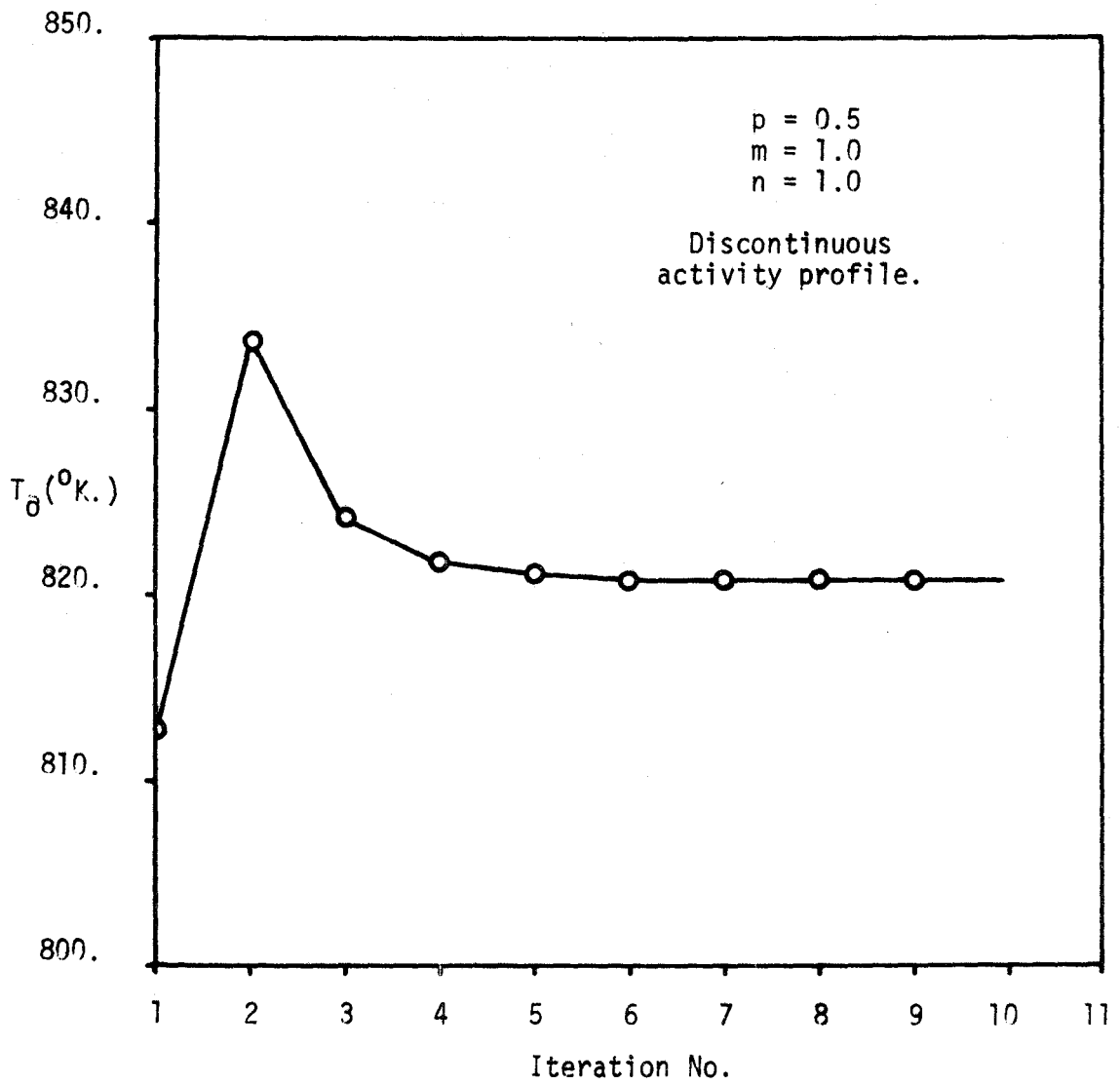

Figure 6-5 Typical Rate Of Convergence Of The Initial Uniform Temperature Along The z Axis For Algorithm S2.

policy for $n > 0$ may however not raise the temperature (hence the rate $k[T]$) everywhere as high as possible, as discussed in section 5.4. This is for example true for values of $n = 0.5$, 1.0 and 2.0 where according to property 9 for $p > 1$ the optimal control surface $k^{+}(z,t)$ defined on τ consists only of controls k^{*} and k_{*}. Extremal control switching lines, which are defined in the plane of τ, bound disjoint regions on τ upon which the controls k^{*} and k_{*} are defined respectively, as illustrated in figure 6-6. For each case taken separately the region contained by the contour $t_0t_1z_1z_0$ ($n = 0.5$) or $t_0t_2z_2z_0$ ($n = 1.0$) or $t_0t_3z_3z_0$ ($n = 2.0$) is one on which the control k_{*} is defined with the control k^{*} defined on the remaining surface in τ. It is observed that as n decreases in value the surface on which the control k_{*} is defined decreases in area, which is consistent with property 10 at the limit for $n \to 0$.

For $p < 1$ and when a stationary policy may exist, the effect of different values of the reaction order on the resulting extremal control policies would be expected to be less significant than for $p > 1$ since the stationary control is continuously variable in both space and time of τ. The effect of considering values of $n = 0.5$, 1.0 and 2.0 on the extremal stationary control policies is illustrated in figure 6-7 where, using sub-property 8 a for a first-order catalyst deactivation process, uniform temperature $T(z,t) = T(t)$, $^{o}K.$, is plotted with time.

6.3.2. Deactivation Order m

For an identical set of operating temperature and initial catalyst activity the magnitude of non-zero catalyst activity at any given time $t > 0$ is greater with larger deactivation order m, as illustrated in figure 6-8.

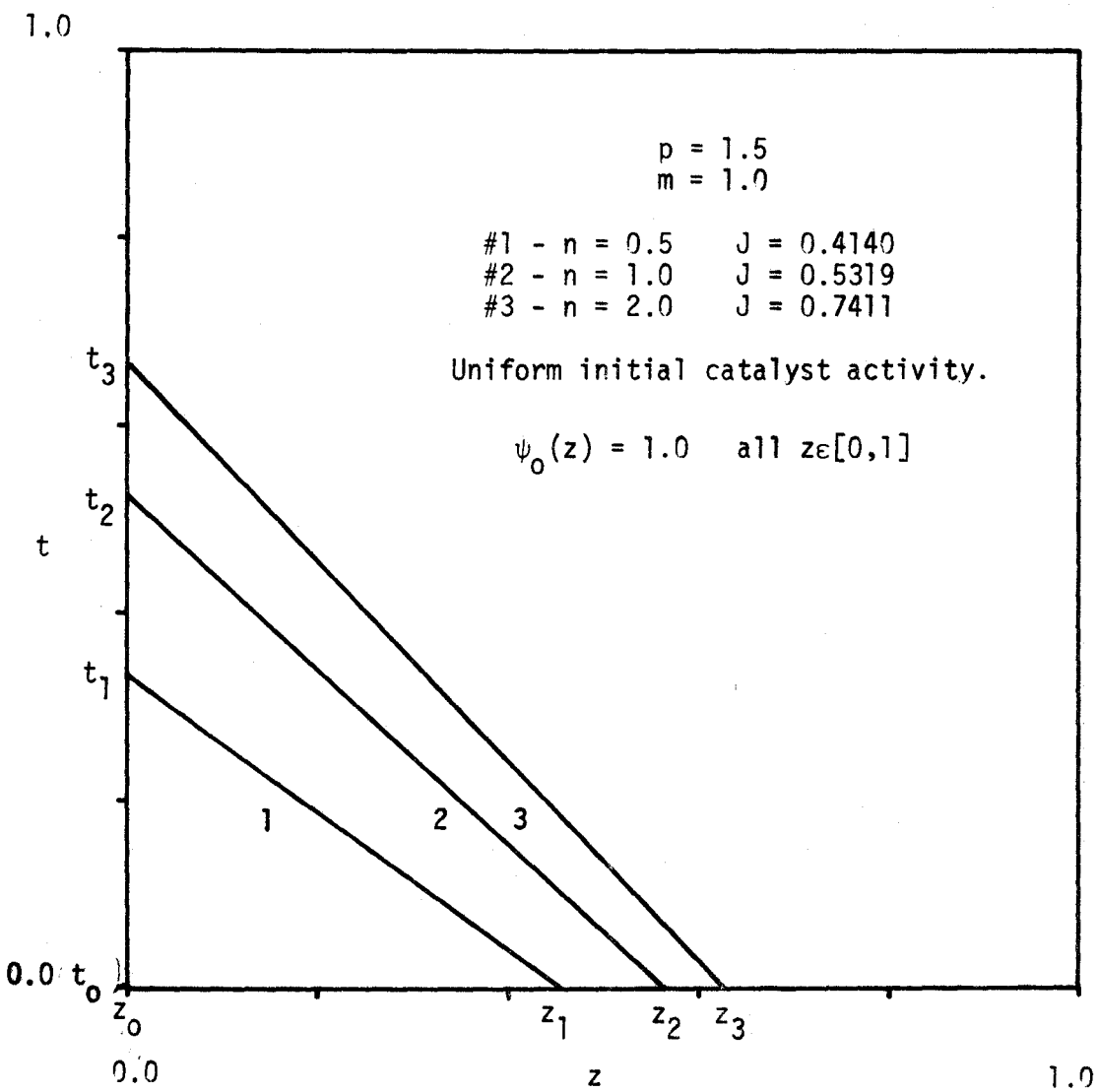

Figure 6-6 Effect Of The Reaction Order n On The Extremal Control Switching Line In The Plane Of Z^o x T^o.

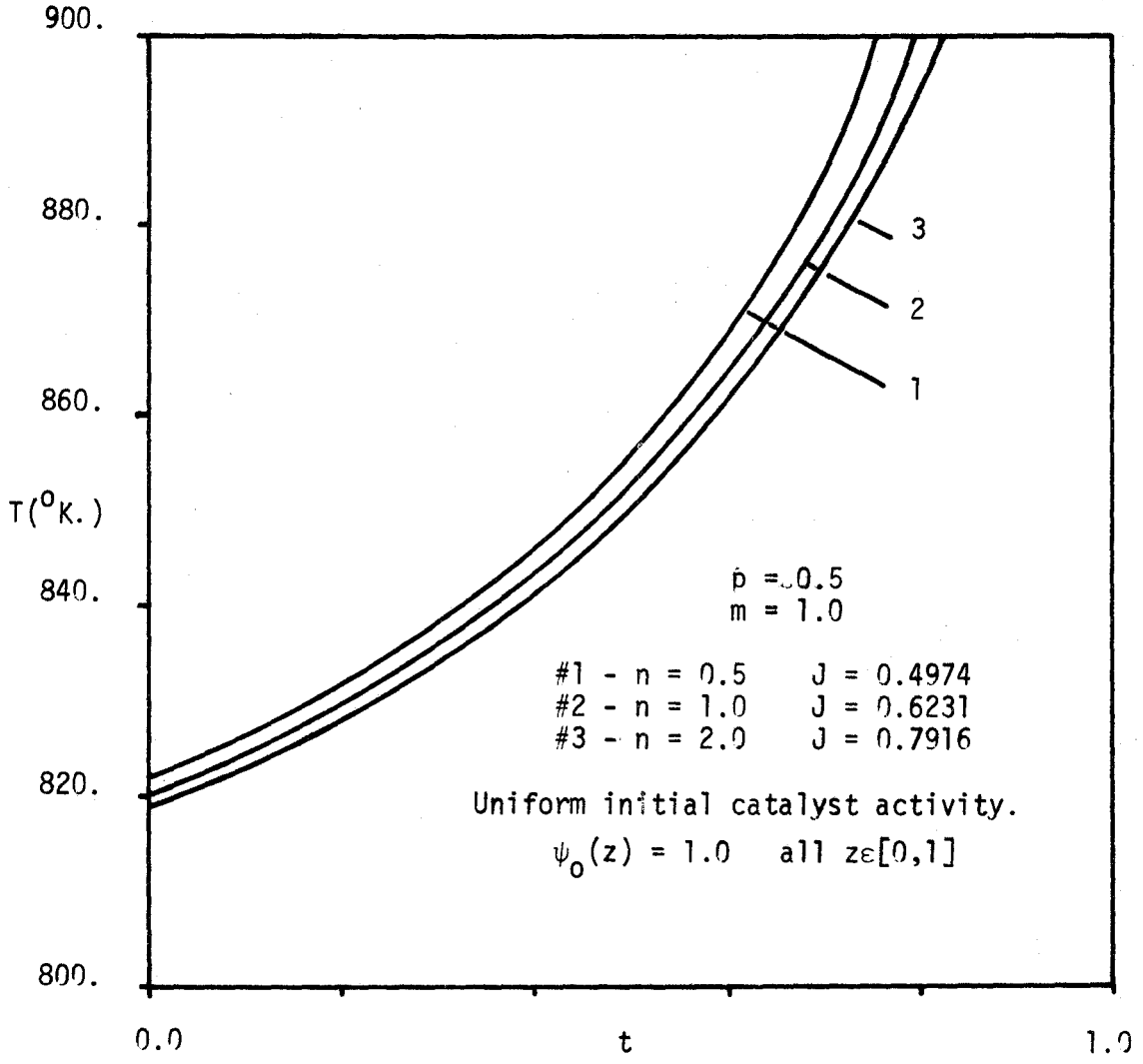

Figure 6-7 Effect Of The Reaction Order n On The Stationary Temperature Policy In Time But Uniform Everywhere In the Reactor.

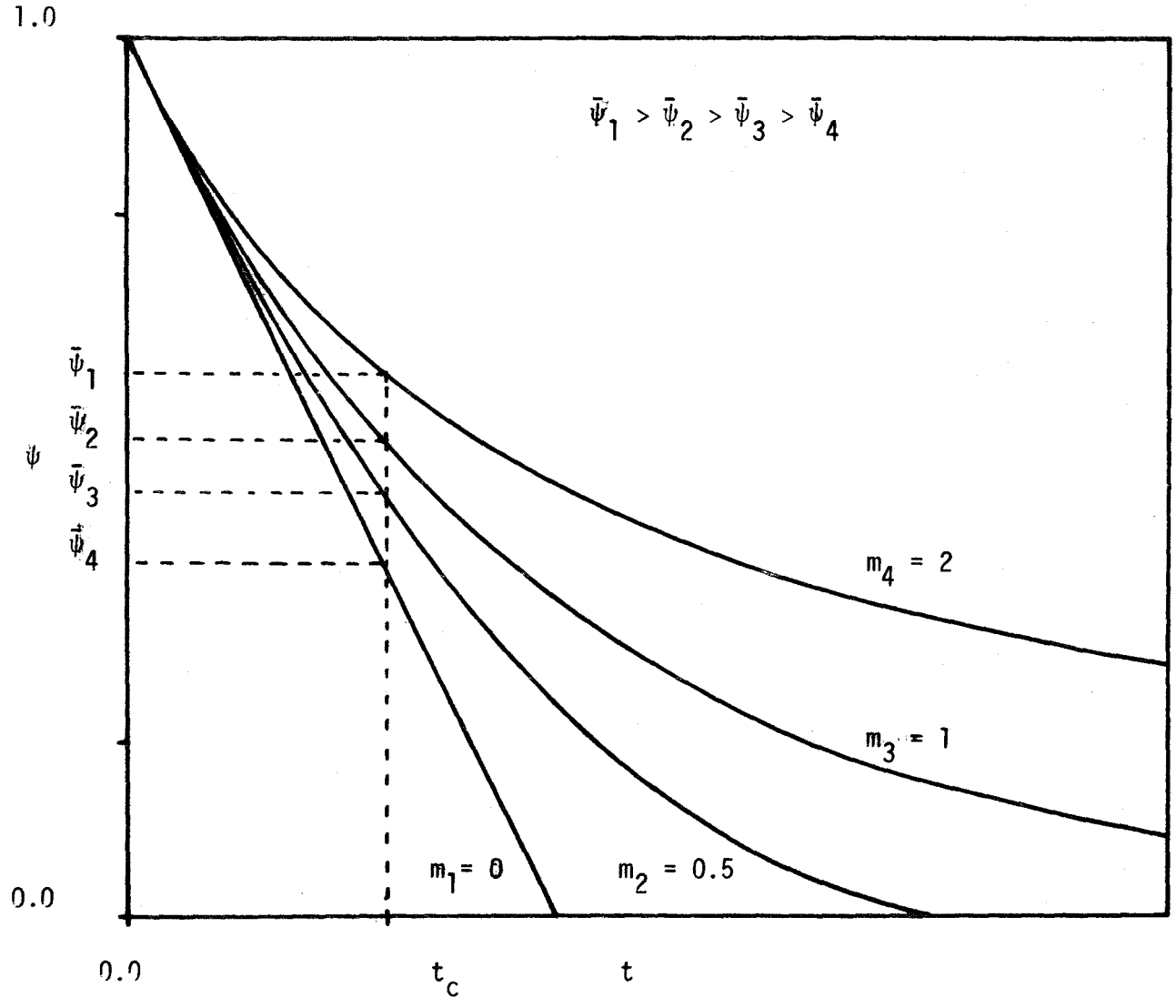

Figure 6-8 Catalyst Activity Profiles In Time Corresponding To Different Deactivation Orders m With Constant Temperature.

The ratio of catalyst decay rates for orders of deactivation $m_1 > m_2$ may be written using equation (3-32),

$$\frac{\text{rate } [T_1,\psi_1,m_1]}{\text{rate } [T_2,\psi_2,m_2]} = \frac{k[T_1].\psi_1^{m_1}}{k[T_2].\psi_2^{m_2}} \qquad (6\text{-}20)$$

and for catalyst activities $1 > \psi_1 \geq \psi_2 \geq 0$ the rate of catalyst decay of the higher order m_1 deactivation process at fixed finite positive temperatures $T_1 = T_2$ is smaller than the rate of catalyst decay for the lower order m_2 deactivation process.

Therefore for identical decay rates with $m_1 > m_2$ and $1 \geq \psi_1 \geq \psi_2 > 0$

$$k[T_1] > k[T_2] \qquad (6\text{-}21)$$

and the temperature T_1 for the higher order m_1 deactivation process is greater than for the lower order m_2 deactivation process.

This would then suggest that the average level of optimal operating temperature of a higher order deactivation process could be at any time higher than that of a lower order deactivation process.

This has been shown to be the case and is illustrated in figure 6-9 for $p > 1$ with values of $m = 1.0$, 1.5 and 2.0 and in figure 6-10 for $p < 1$ with values of $m = 0.75$, 1.0 and 2.0.

6.3.3. Parameter $p = E_R/E_c$

The role of the parameter p in the admissibility of a control sub-policy S, C_* or C^* to an optimal control policy has been discussed in chapter 5.

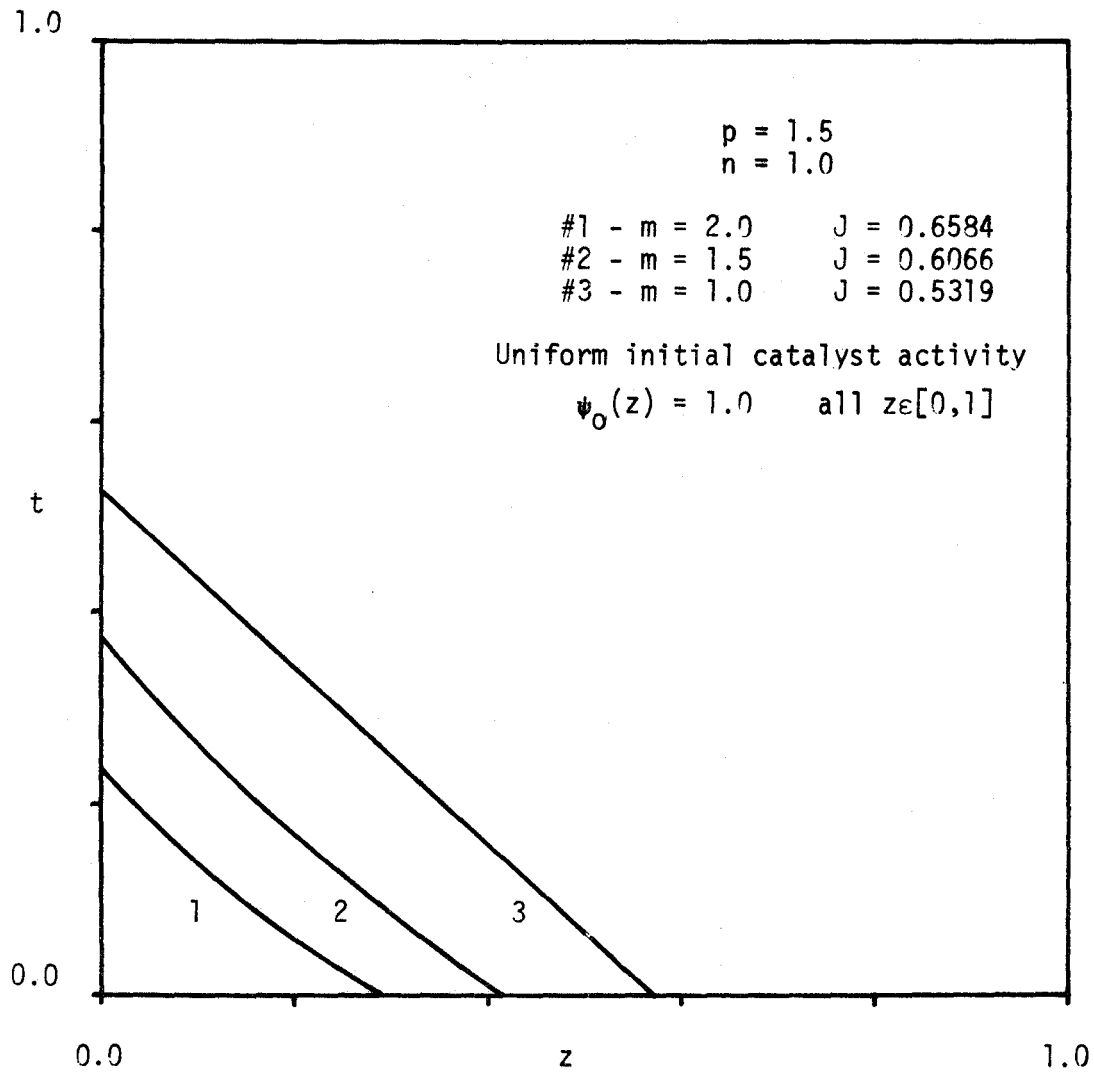

Figure 6-9 Effect Of The Catalyst Deactivation Order m On The Extremal Control Switching Line In The Plane Of Z^o x T^o.

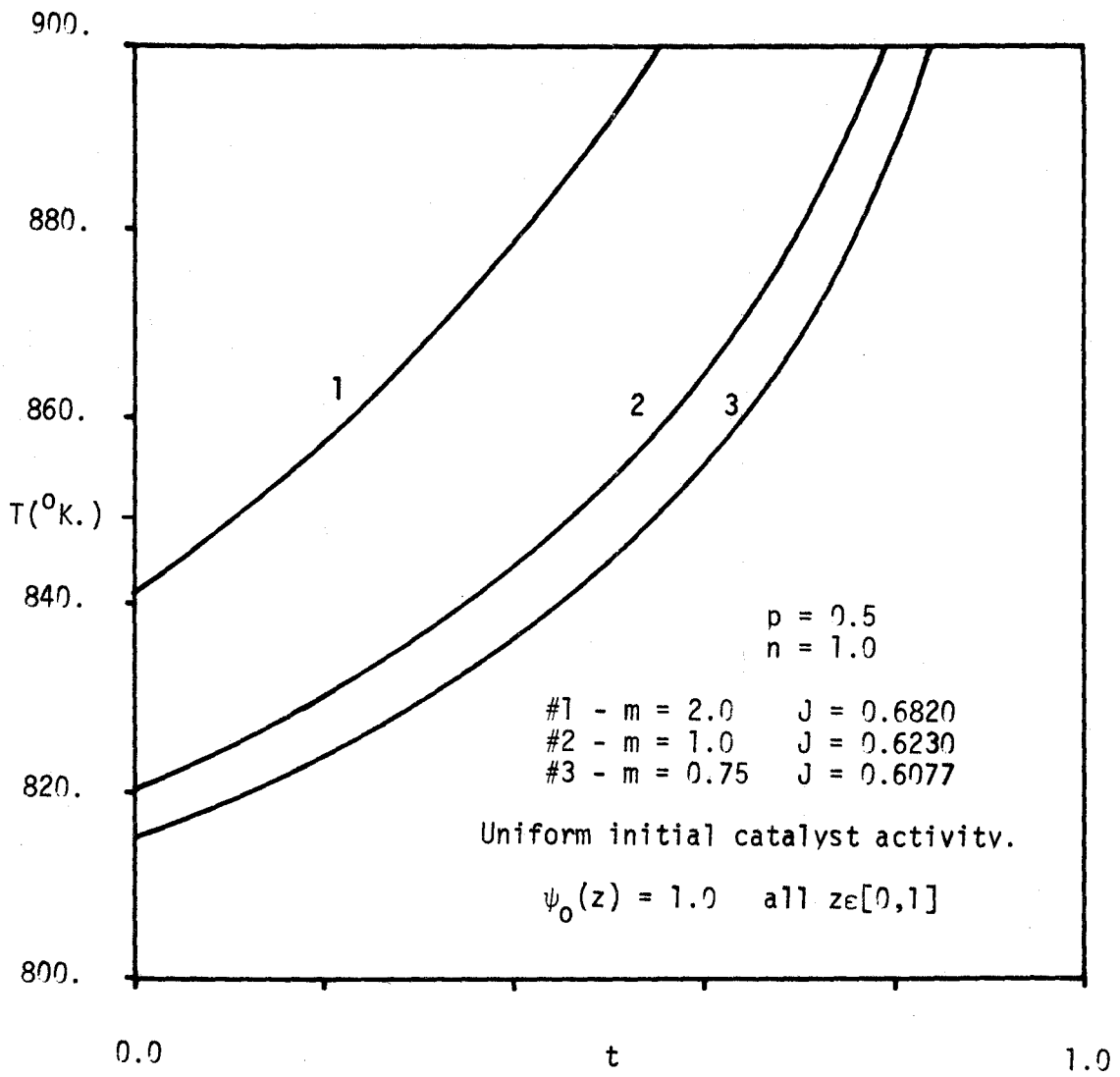

Figure 6-10 Effect Of The Catalyst Deactivation Order m On The Stationary Temperature Policy In Time But Uniform Everywhere In The Reactor.

For a value of p = 0 the reaction rate is independent of temperature and as low a temperature (hence k[T]) as possible should be chosen in order to retain the highest possible catalyst activity in the reactor. For p = ∞ the deactivation rate is virtually independent of the temperature and as high as temperature as possible should be chosen in order to achieve the highest possible conversion level.

This would suggest that to higher values of p > 0 correspond higher average level of temperature in the reactor. This is observed for 0 < p < 1, namely for the values of p = 0.1, 0.5 and 0.9 where the significant effect on the extremal stationary control policy is illustrated in figure 6-11. However for p > 1, namely for the values of p = 1.1, 1.5, 2.5 and 5.0 the effect on the resulting extremal control switching lines is nearly indistinguishable when plotted on the z-t plane and results are shown in table 6-2. The tabulation contains results considering a first and second-order catalyst deactivation processes (m = 1, m = 2) and the intercepts of the control switching line with the coordinate t axis (z = 0) and z axis (t = 0) in the plane of τ are given for each case. Although the surface area where the control k_* is defined only slightly diminishes with increasing finite values of p, nevertheless, it indicates that for the range of p considered (very far from p = ∞) the average level of temperature in the reactor very slowly increases with higher values of p.

In contrast with the results for 0 < p < 1 where the effect of different values of p on the resulting exit conversion X(1,t) profile in time is very significant, the results for p > 1, p = 1.1, 1.5, 2.5 and 5.0, shows indistinguishable exit conversion profiles X(1,t) when plotted in figure 6-12. Values for the initial and terminal exit conversion assessing the small changes in these profiles for p > 1 are listed in table 6-2. A measure of the amount

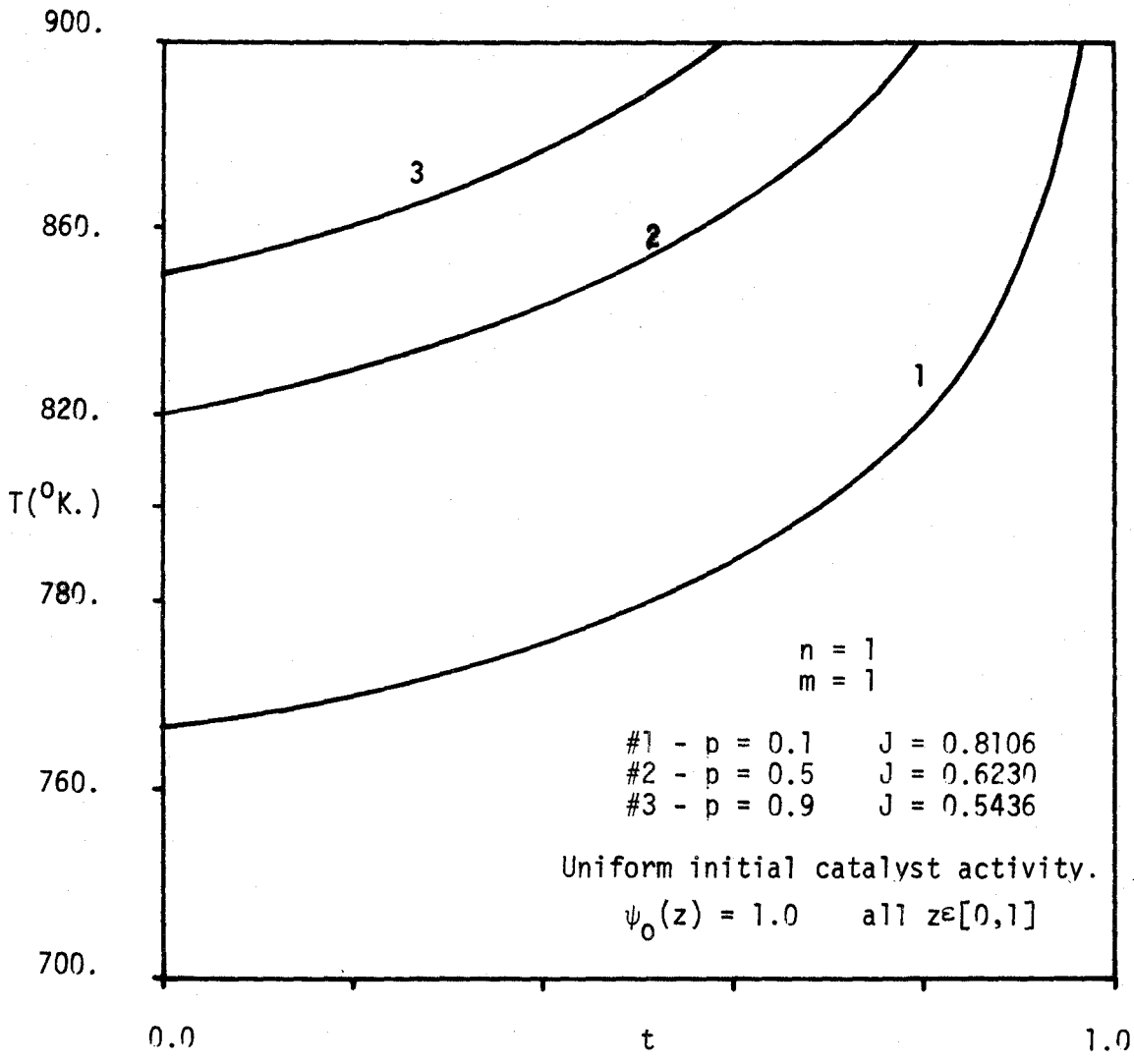

Figure 6-11 Effect Of The Kinetic Parameter p On The Stationary Temperature Policy In Time But Uniform Everywhere In The Reactor.

$p = \frac{E_R}{E_c}$	Reaction order n	Catalyst decay order m	Control switching line intercept (z = o) t	(t = o) z	Exit conversion initial X(1,0)	terminal X(1,1)	Extremal policy J
1.1	1.0	1.0	.52658	.57312	.62840	.25771	.53244
1.5	1.0	1.0	.52347	.56795	.63060	.25597	.53186
2.5	1.0	1.0	.52295	.56707	.63097	.25569	.53177
5.0	1.0	1.0	.52295	.56706	.63097	.25568	.53176
1.1	1.0	2.0	.24010	.28735	.8069	.4878	.65848
1.5	1.0	2.0	.23711	.28360	.8080	.4876	.65841
2.5	1.0	2.0	.23660	.28296	.8082	.4876	.65840

Table 6-2 Effect Of The Kinetic Parameter p For A First And Second Order Catalyst Deactivation On The Intercept Of The Extremal Control Switching Lines With The t and z Axis, The Initial And Terminal Conversion And The Amount of Reaction J.

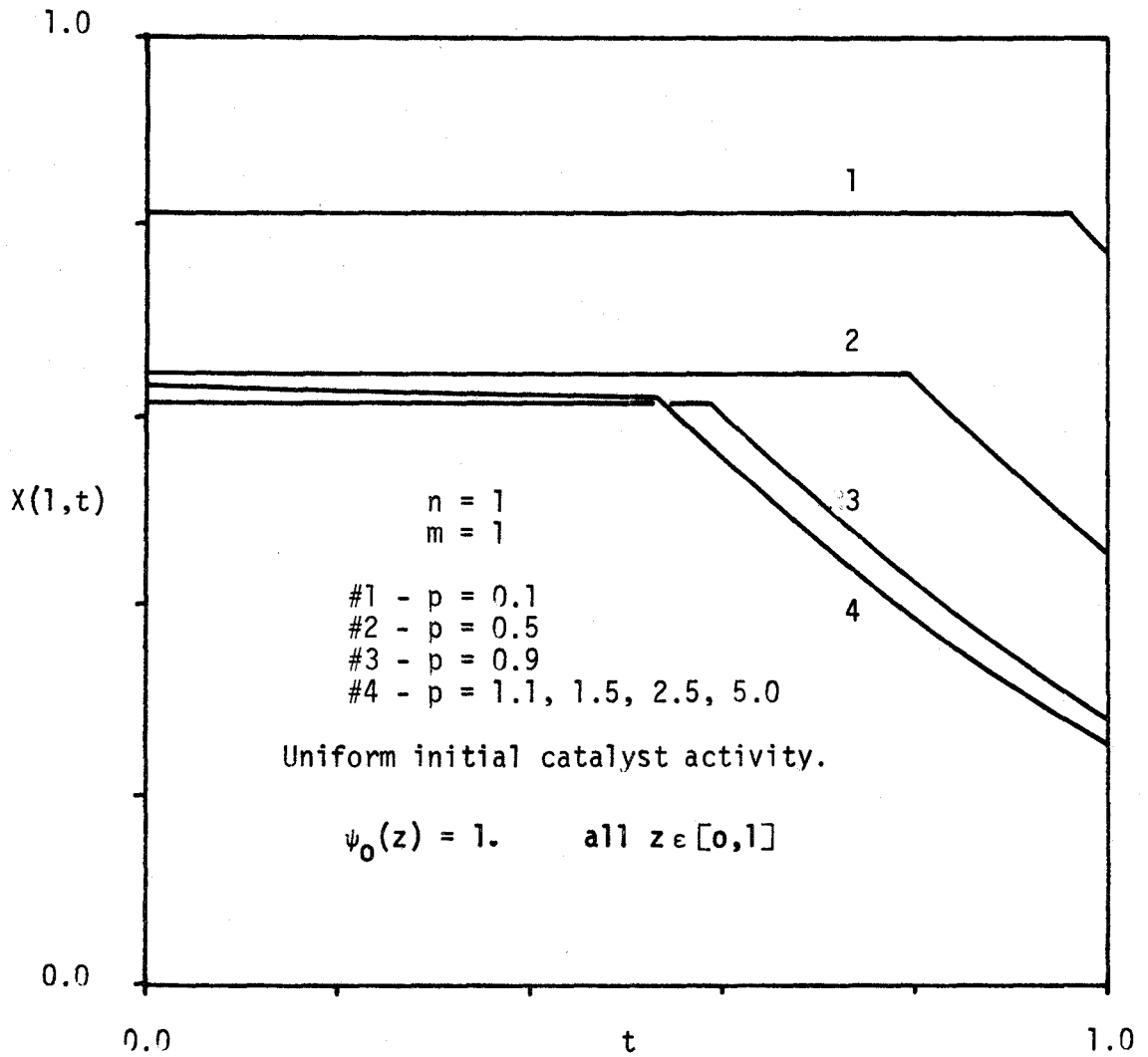

Figure 6-12 Effect Of The Kinetic Parameter p On The Extremal Exit Conversion X(1,t) Profiles With Time.

of reaction J resulting from such extremal control surface and computed by equation (3-41) is also given there for $p > 1$, and a comparative illustration of that measure with the case of $0 < p < 1$ is given in figure 6-13.

6.4. Catalyst Activity Profiles and the Order of Deactivation

6.4.1. Stationary Control Policies

A continuous exponentially increasing initial catalyst activity profile,

$$\psi_o(z) = (0.75).\exp\{(0.28765).z\} \qquad z \in [0.1] \tag{6-22}$$

and a piecewise uniform catalyst initial activity profile,

$$\begin{aligned} \psi_o(z) &= 1.0 && z \in [0.0.5] \\ \psi_o(z) &= 0.8 && z \in (0.5,1.0] \end{aligned} \tag{6-23}$$

and their relative effect on the extremal stationary control policy S for a first and second-order catalyst deactivation process are considered.

Since for a first-order catalyst deactivation process properties 8 and 8a hold, the extremal control $\hat{k}(z,t)$ in time is uniform along the entire length of the reaction irrespective of the uniformity or continuity of the catalyst activity distribution along the reactor length. These properties of the extremal stationary control policy S have been observed for $m = 1$ and are illustrated in figure 6-14 for the continuous non-uniform catalyst activty profile (6-22)

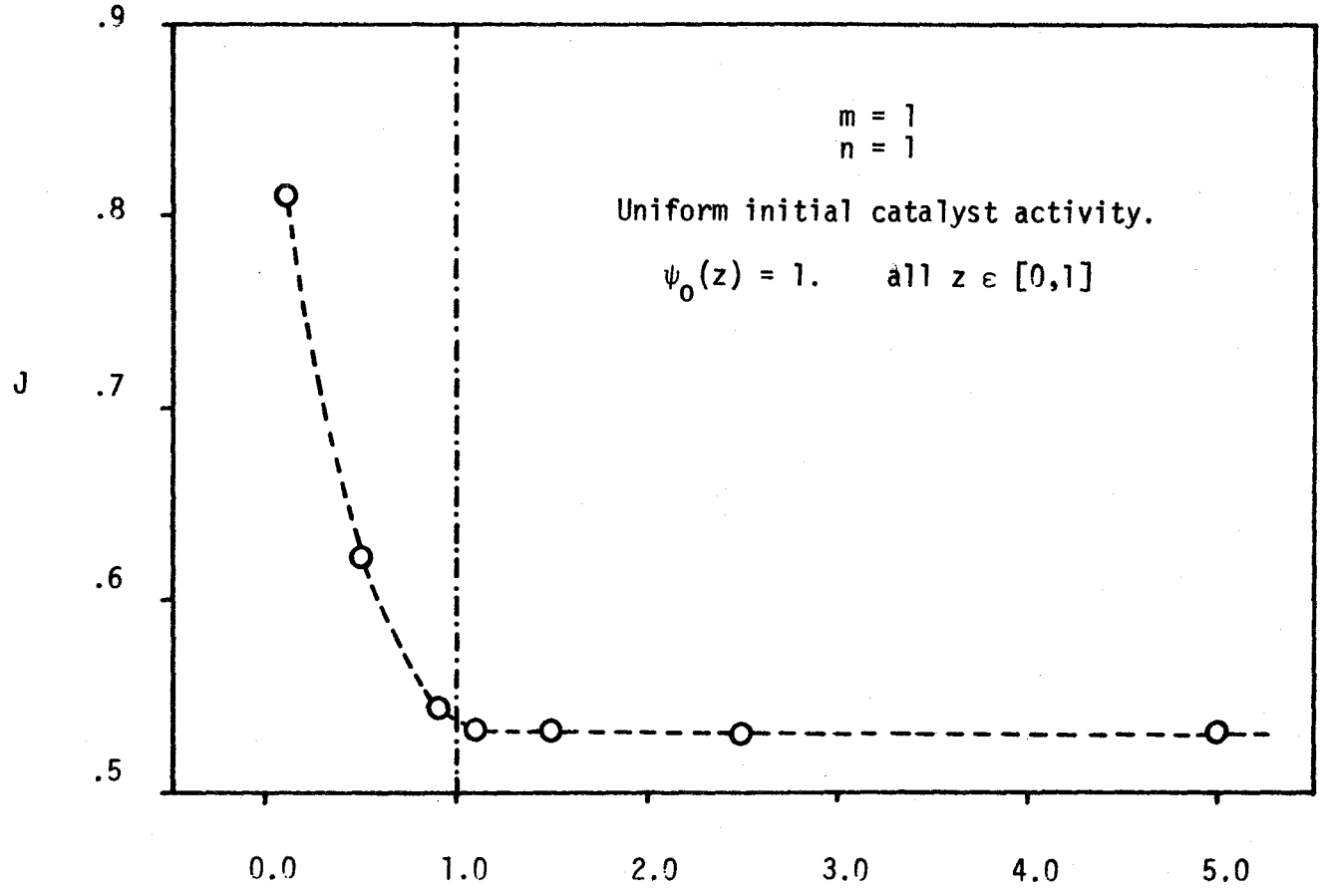

Figure 6-13 Effect Of The Kinetic Parameter p On The Amount Of Reaction J Produced.

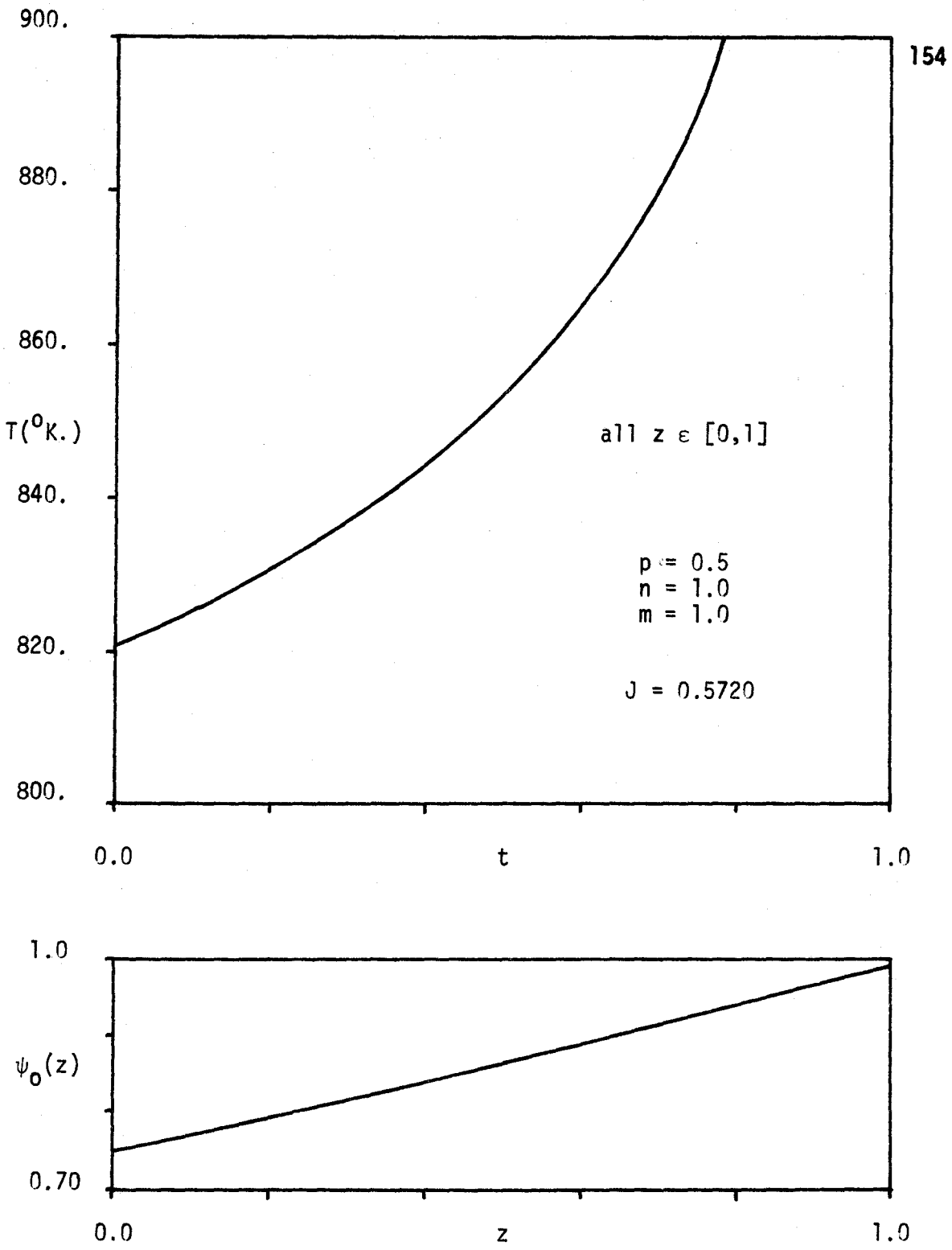

Figure 6-14 Effect Of A Continuous Non-Uniform Initial Catalyst Activity On The Extremal Stationary Temperature Policy In Time For A First-Order Deactivation Process.

and in figure 6-15 for the discontinuous but piecewise uniform catalyst activity profile (6-23).

However, for a second-order catalyst deactivation process the extremal control $\hat{k}(z,t)$ is sensitive to both the uniformity and continuity of the catalyst activity profile along the reactor length.

This observation is illustrated in figure 6-16 and 6-17 respectively for catalyst distributions (6-22) and (6-23) where no longer is the extremal stationary control policy S uniform for a non-uniform catalyst activity profile or continuous for a discontinuous catalyst activity profile.

6.4.2. Bang-bang Control Policies

A piecewise uniform initial catalyst activity profile,

$$\begin{aligned} \psi_0(z) &= 1.0 \qquad && z \in [0.0,0.2] \\ \psi_0(z) &= 0.90 \qquad && z \in (0.2,1.0] \end{aligned} \tag{6-24}$$

and its relative effect on the extremal control switching line for a first and second-order catalyst deactivation process are considered.

The case of a first-order catalyst deactivation process is discussed in section 5.4.1. and it is shown that a necessary and sufficient condition (5-177) defining an extremal control switching line in τ is independent of the uniformity or continuity of the catalyst activity distribution along the length of the reactor. The result illustrated in figure 6-18 establishes this fact.

For a second-order catalyst deactivation process, however, the control switching line in τ is sensitive to a discontinuity in the initial catalyst

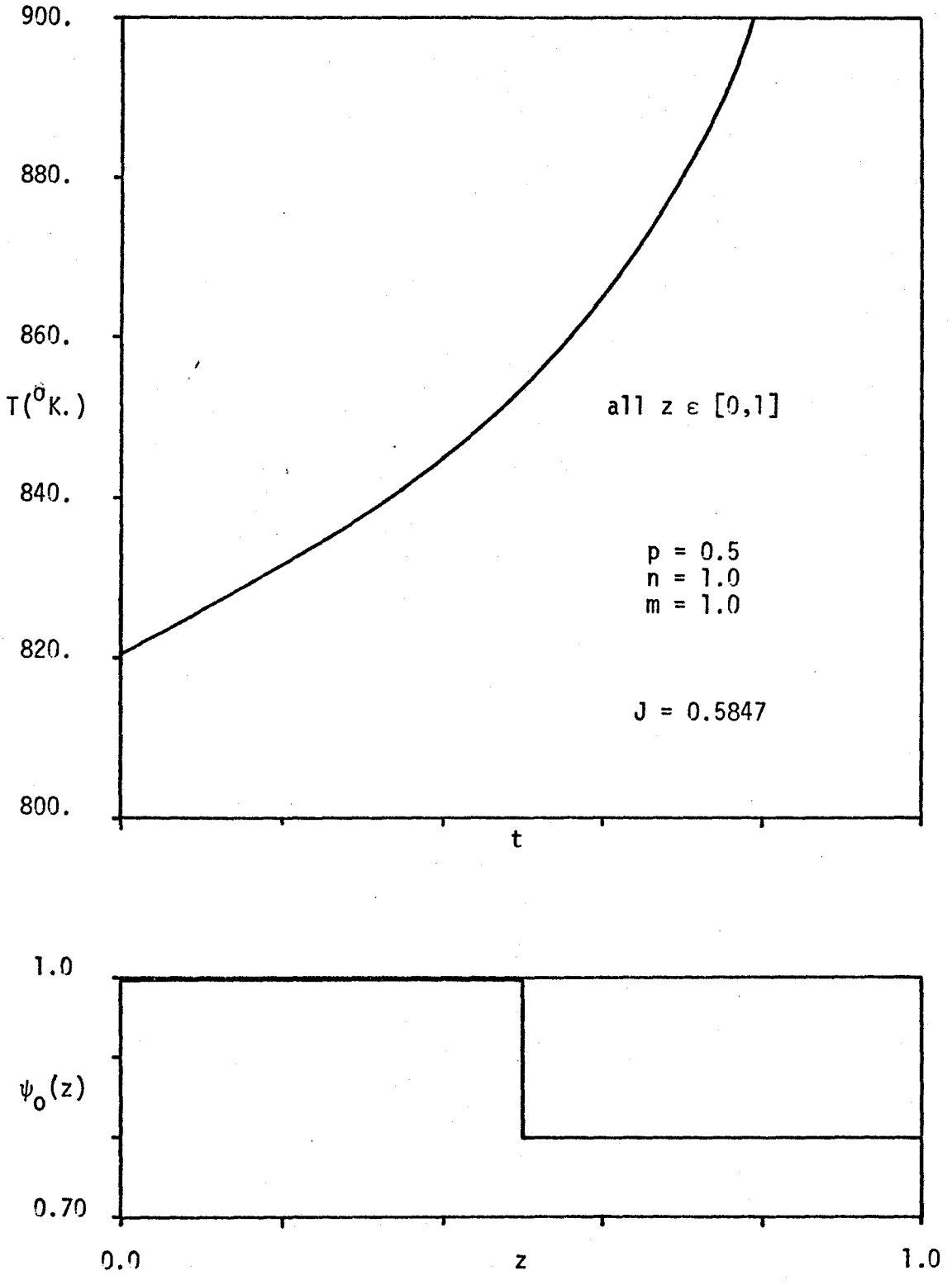

Figure 6-15 Effect Of A Discontinuous Uniform Initial Catalyst Activity On The Extremal Stationary Temperature Policy In Time For A First-Order Deactivation Process.

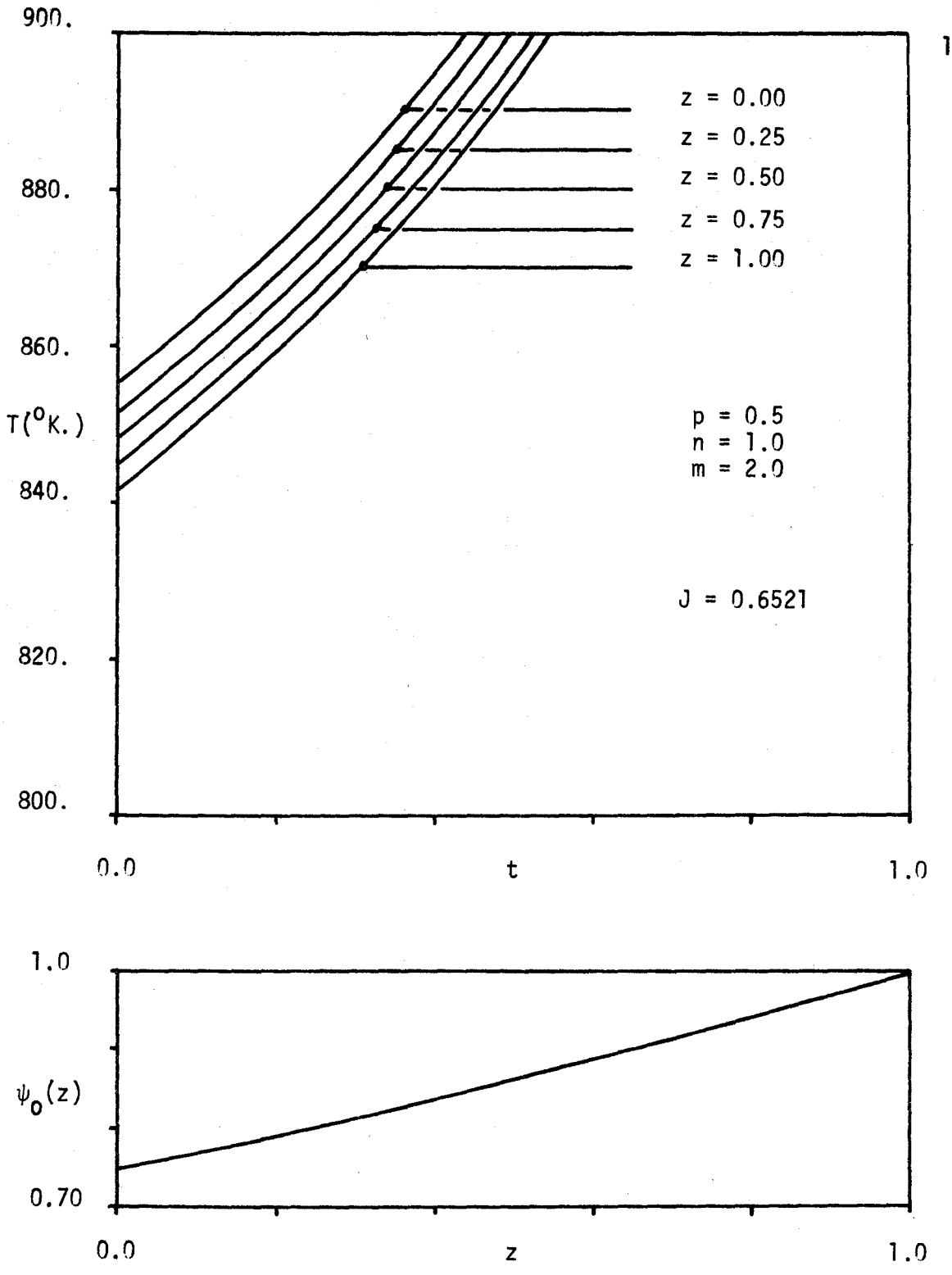

Figure 6-16 Effect Of A Continuous Non-Uniform Initial Catalyst Activity On The Extremal Stationary Temperature Policy In Time For A Second-Order Deactivation Process.

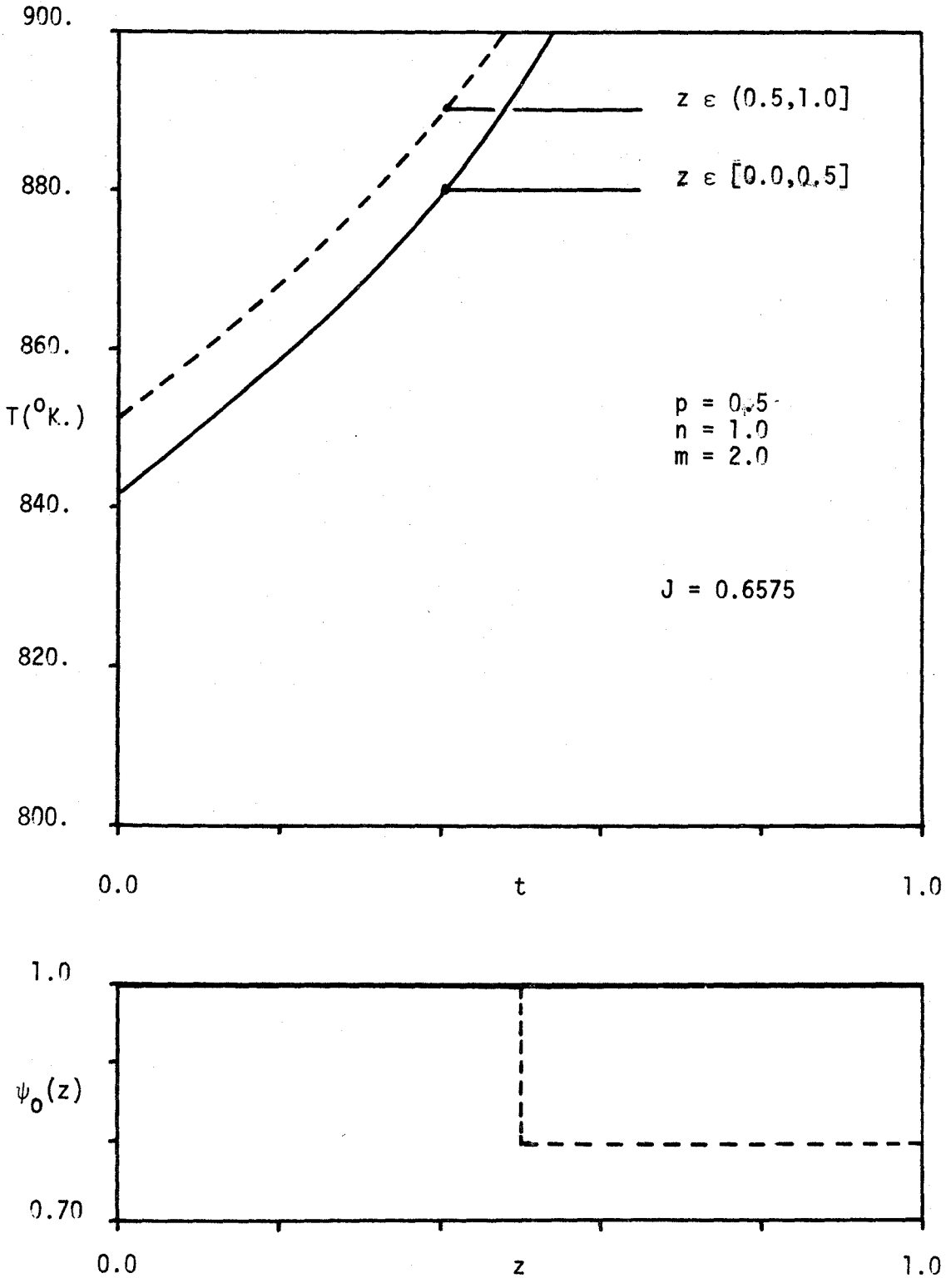

Figure 6-17 Effect Of A Discontinuous Uniform Initial Catalyst Activity On The Extremal Stationary Temperature Policy In Time For A Second-Order Deactivation Process.

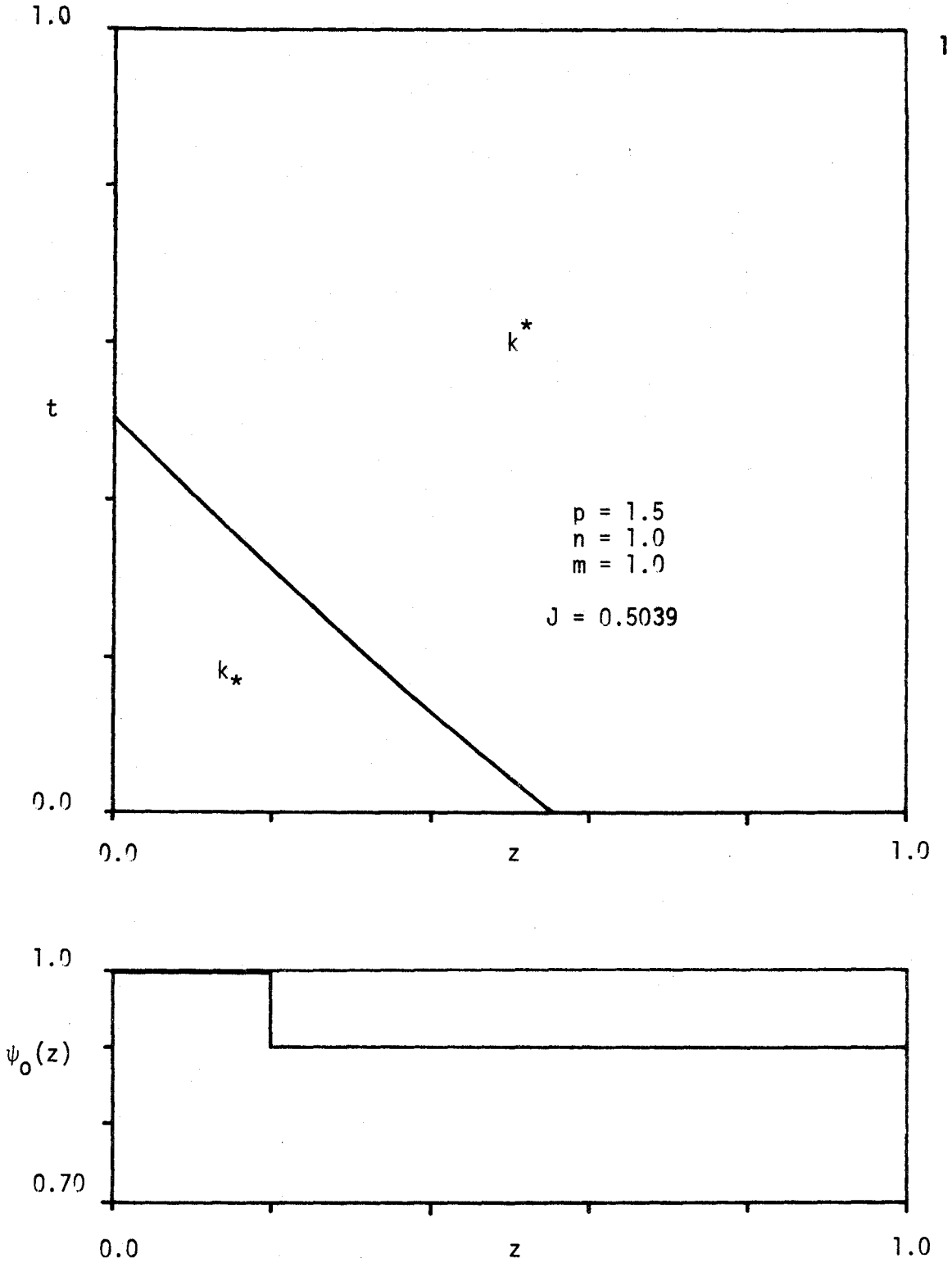

Figure 6-18 Effect Of A Discontinuous Uniform Initial Catalyst Activity On The Extremal Control Switching Line In The Plane Of Z^{o} x T^{o} For A First-Order Deactivation Process.

activity profile. This is reflected in figure 6-19 where for illustration the first iterative steps of algorithm C1 are shown starting with an initial pseudo-extremal continuous control switching line in τ. The generation of a pseudo-extremal discontinuous control switching line developed at the second iteration and remained thereafter at the point of discontinuity of the initial catalyst activity profile.

6.4.3. Catalyst Activity Distributions

The distribution of an initial catalyst change according to different activity profiles along the length of the reactor but with an identical average activity level,

$$\psi_{mean} = \int_0^1 \psi_0(z).dz \qquad (6\text{-}25)$$

is considered. The following distributions are used,

$$\text{case 1} \quad \psi_0(z) = 0.869 \qquad z \in [0,1] \qquad (6\text{-}26)$$

$$\text{case 2} \quad \psi_0(z) = 1.0 \qquad z \in [0.0,0.5]$$

$$\psi_0(z) = 0.738 \qquad z \in (0.5,1.0] \qquad (6\text{-}27)$$

$$\text{case 3} \quad \psi_0(z) = (0.75).\exp\{(0.28765).z\} \qquad z \in [0,1] \qquad (6\text{-}28]$$

with $\psi_{mean} = 0.869$ in each case.

The effect of these different activity profiles on the extremal control switching lines is illustrated in figure 6-20 for a first-order catalyst

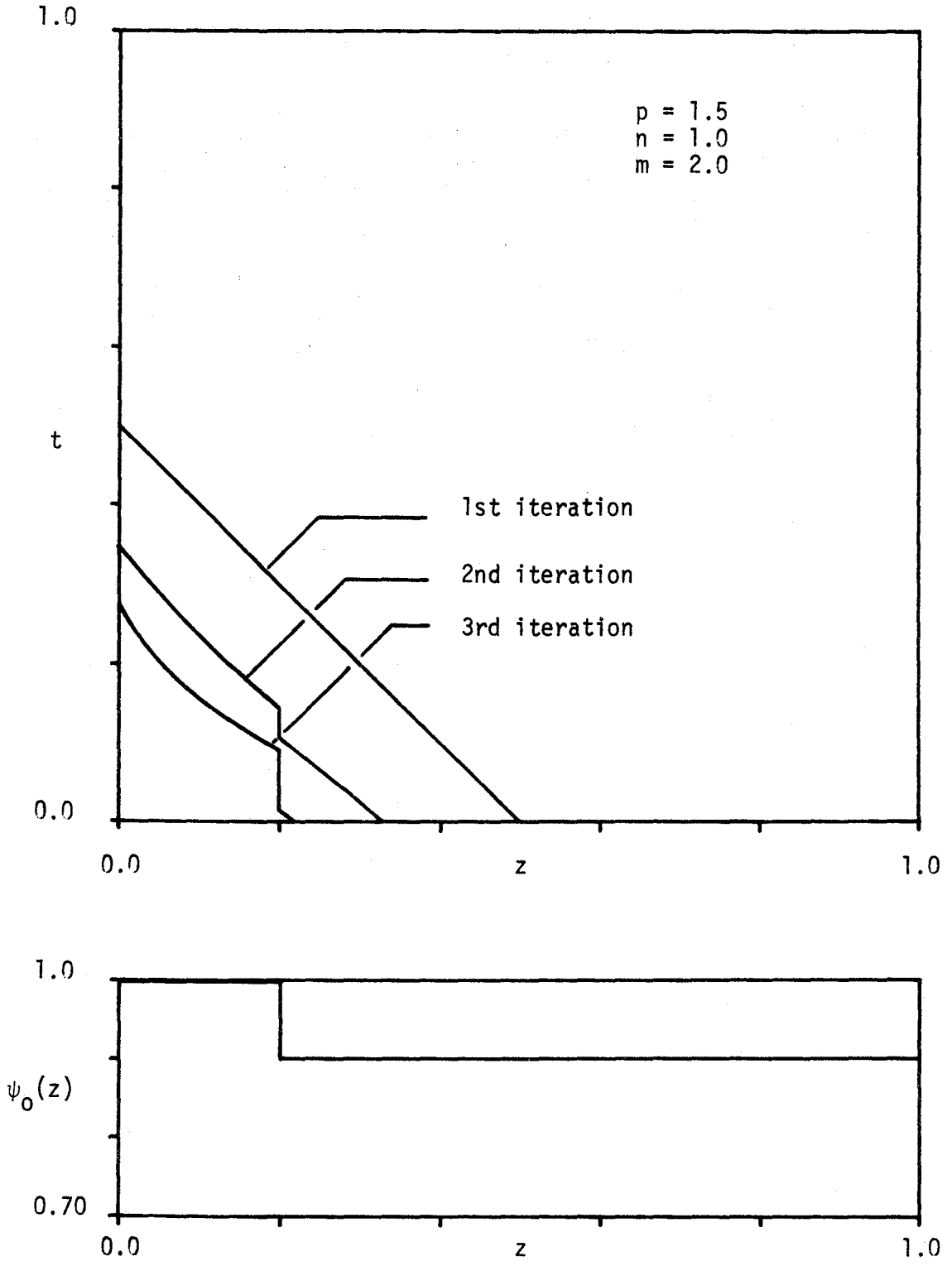

Figure 6-19 Effect Of A Discontinuous Uniform Initial Catalyst Activity On The Extremal Control Switching Line In The Plane Of Z^o x T^o For A Second-Order Deactivation Process.

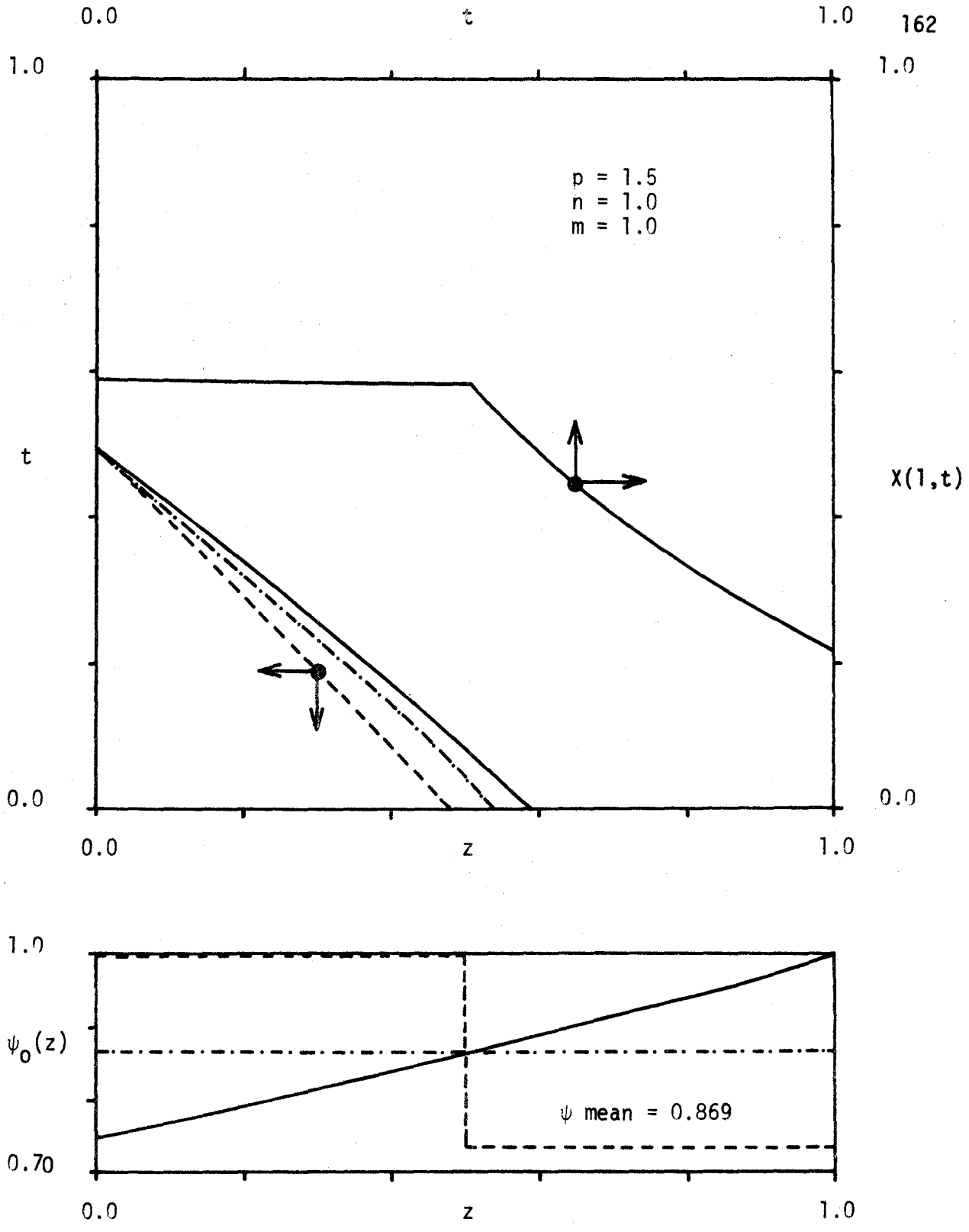

Figure 6-20 Effect Of Various Initial Catalyst Activity Profiles With Mean = 0.869 On The Extremal Control Switching Line And Exit Conversion In Time For A First-Order Deactivation Process.

deactivation process with n = 1 and p = 1.5. The resulting exit conversion X(1,t) profile is identical in all cases and thus the amount of reaction (3-41) produced is the same whatever catalyst activity profile is used.

The effect on the extremal stationary control policy S discussed in section 6.4.1. for m = 1 is also illustrated in figure 6-21 for n = 1 and p = 0.5. Again the amount of reaction produced is invariant towards the use of the catalyst activity profiles (6-26), (6-27) and (6-28).

However when a second-order catalyst deactivation process m = 2 is considered for a first-order reaction with p = 0.5 and corresponding to catalyst activity profiles (6-26), (6-27) and (6-28), the exit conversion X(1,t) profiles although nearly the same in time are no longer identical there. A comparative description of the initial and terminal exit conversion in time with the corresponding amount of reaction (3-41) is given in table 6-3 for both m = 1 and m = 2.

The tabulated results for m = 2 would seem to indicate that an optimal distribution of catalyst activity along the length of the reaction could exist such that with the corresponding extremal control surface the amount of reaction (3-41) be maximized.

Results from figures 6-20 and 6-21 or tabulated for m = 1 would seem to indicate however that this is not the case for a first-order catalyst deactivation process.

6.5. Best Isothermal Operating Policies

A way of assessing the extremal policies identified in this study is to compare them with the best isothermal operating policies (best uniform temperature in both space and time).

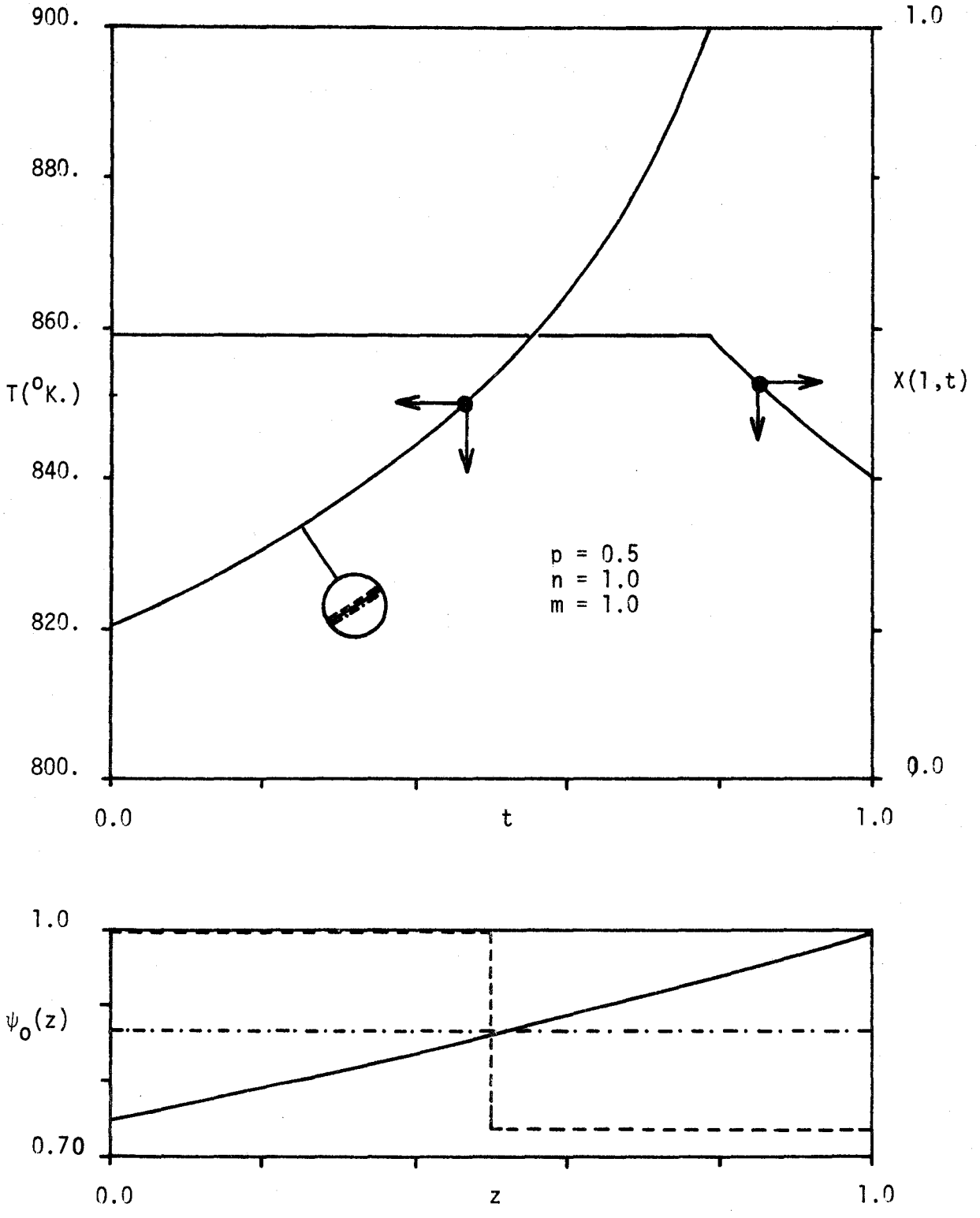

Figure 6-21 Effect Of Various Initial Catalyst Activity Profiles With Mean = 0.869 On The Extremal Stationary Temperature Policy And Exit Conversion In Time For A First-Order Deactivation Process.

Initial catalyst activity profile	$p = \frac{E_R}{E_c}$	Reaction order n	Catalyst decay order m	Exit conversion initial X(1,0)	Exit conversion terminal X(1,1)	Extremal policy J
(6-26)	1.5	1.0	1.0	.5908	.2187	.4850
(6-27)	1.5	1.0	1.0	.5908	.2187	.4850
(6-28)	1.5	1.0	1.0	.5908	.2187	.4850
(6-26)	0.5	1.0	1.0	.5918	.4089	.5720
(6-27)	0.5	1.0	1.0	.5918	.4089	.5720
(6-28)	0.5	1.0	1.0	.5918	.4089	.5720
(6-26)	0.5	1.0	2.0	.6982	.5174	.6501
(6-27)	0.5	1.0	2.0	.6990	.5161	.6496
(6-28)	0.5	1.0	2.0	.6998	.5192	.6520

Table 6-3 Effect Of Various Initial Catalyst Activity With Mean = 0.869 For A First And Second-Order Deactivation Process With p = 0.5 and p = 1.5 On The Initial And Terminal Exit Conversion And Amount Of Reaction J Produced.

Results were obtained for different sets of kinetic parameters p, n and m and the following types of catalyst activity profiles,

$$\text{type 1:}\quad \psi_0(z) = 1. \qquad \text{all } z \in [0,1] \tag{6-29}$$

$$\text{type 2:}\quad \psi_0(z) = 0.869 \qquad \text{all } z \in [0,1] \tag{6-30}$$

$$\text{type 3:}\quad \psi_0(z) = (0.75),\exp\{(0.28765).z\} \qquad \text{all } z \in [0,1] \tag{6-31}$$

$$\text{type 4:}\quad \begin{aligned} \psi_0(z) &= 1.0 && z \in [0.0,0.5] \\ \psi_0(z) &= 0.9 && z \in (0.5,1.0] \end{aligned} \tag{6-32}$$

$$\text{type 5:}\quad \begin{aligned} \psi_0(z) &= 1.0 && z \in [0.0,0.5] \\ \psi_0(z) &= 0.8 && z \in (0.5,1.0] \end{aligned} \tag{6-33}$$

Tables 6-4 and 6-5 summarized these results. The relative improvement in the amount of reaction (3-41) J and J_I for the extremal distribution control policy over the more conservative best isothermal operating policy is also given.

Although an improvement over the best isothermal operating policy has been noticed in all cases studied, tabulated results indicated that a greater gain would be achieved for first-order than second-order catalyst deactivation processes for both values of p = 0.5 and p = 1.5.

This is found compatible with the arguments contained in section 6.3.2. since as m increases a higher level of temperature would be used and for $m \to \infty$ an extremal control policy could result for $0 < p < \infty$ in a purely k^* policy hence corresponding to the best isothermal control policy k^* with a relative improvement zero.

$p = \frac{E_R}{E_c}$	Reaction order n	Catalyst decay order m	Initial catalyst activity $\psi_o(z)$	Extremal policy J	Isothermal policy J_I	$\frac{J - J_I}{J}$
1.5	1.0	1.0	Type 1	.5318	.5022	+ 5.57
1.5	1.0	1.5	"	.6066	.5992	+ 1.23
1.5	1.0	2.0	"	.6584	.6569	+ 0.23
1.5	0.5	1.0	"	.4139	.4069	+ 1.69
1.5	2.0	1.0	"	.7411	.6970	+ 5.95
1.5	1.0	1.0	Type 3	.4850	.4654	+ 4.04
1.5	1.0	1.0	Type 4	.5038	.4782	+ 5.08

Table 6-4 Relative Improvement Of The Distributed Control Policy Over The Best Isothermal Policy For p = 1.5 And Various Combinations Of The Reaction Order n, Deactivation Order m, And Initial Catalyst Activity Profiles.

$p = \frac{E_R}{E_c}$	Reaction order n	Catalyst decay order m	Initial catalyst activity $\psi_o(z)$	Extremal policy J	Isothermal policy J_I	$\frac{J - J_I}{J}$
0.5	1.0	0.75	Type 1	.6076	.5724	+ 5.79%
0.5	1.0	1.0	"	.6230	.5865	+ 5.85%
0.5	1.0	2.0	"	.6819	.6570	+ 3.65%
0.5	0.5	1.0	"	.4974	.4655	+ 6.42%
0.5	2.0	1.0	"	.7915	.7709	+ 2.60%
0.5	1.0	1.0	Type 2	.5720	.5376	+ 6.00%
0.5	1.0	2.0	"	.6501	.6324	+ 2.71%
0.5	1.0	1.0	Type 3	.5720	.5418	+ 5.27%
0.5	1.0	2.0	"	.6520	.6341	+ 2.75%
0.5	1.0	1.0	Type 5	.5846	.5497	+ 5.97%
0.5	1.0	2.0	"	.6574	.6378	+ 3.00%

Table 6-5 Relative Improvement Of The Distributed Control Policy Over The Best Isothermal Policy For p = 0.5 And Various Combinations Of The Reaction Order n, Deactivation Order m, And Initial Catalyst Activity Profiles.

For $p = 1.5$, a similar but opposite pattern is recognizable from the tabulated data since for n decreasing the relative improvement of J over J_I is decreasing. This behaviour is again consistent with the discussion given in section 6.4.1. since for $p > 1$ and as $n \to 0$ an extremal control policy would tend towards a purely k^* policy and would then correspond at the limit for $n \to 0$ to the best isothermal control policy k^* with a relative improvement zero.

However for $p < 1$ since for decreasing n or even $n = 0$ raising the temperature would not increase the rate constant K[T] for reaction faster than the rate constant k[T] for decay an extremal control policy would not be expected in general to be purely k^* there and the above arguments are not valid in this case.

Therefore a significant improvement of the extremal distributed control policy over the best isothermal control policy in the amount of reaction produced may be expected in general for low order catalyst deactivation processes and with high order reaction systems for $p > 1$.

CHAPTER 7

SUMMARY AND CONCLUSIONS

The maximum principle formulation of Sirazetdinov and Degtyarev (1967) derived for unsteady-state processes has been applied to a quasi-steady state catalytic reaction-deactivation system. The problem of choosing a temperature policy as a function of chronological time and position in a tubular fixed-bed, one-dimensional flow reactor so as to maximize the total amount of reaction in a fixed period of time has been solved. A single irreversible reaction with a rate expressible as a product of separate functions of temperature, activity and conversion was considered with a rate of decay also expressible as a product of separate functions but independent of conversion.

Analytical identification of properties of the optimal policy were given with proofs. The role of the parameter $p = E_R/E_c$ in the admissibility of a control sub-policy S, C_* or C^* to an optimal control policy is also indicated.

It is shown that for all $o < p < \infty$ the optimal temperature everywhere in the reaction is T^* over a terminal time interval, unless the catalyst activity $\psi(z,t)$ along finite portions of the reactor is zero, in which case the rate of reaction is invariant to a change in the current temperature policy there, or unless the conversion level $X(z,t)$ in the reactor is unity, that is $F[X] = 0$, and where there is clearly no incentive in choosing a temperature higher than that required to maintain $X(z,t) = 1$.

For $o < p < 1$, it is shown that at each and every point of the reactor an optimal temperature policy $T^{+}(z,t)$ in time, corresponding to a continuous monotonic non-increasing inlet conversion $X_o(t)$ in time, is a continuous monotonic non-decreasing function of time and may consist only of the following control policies: $\{T^{*}\}$, $\{S \rightarrow T^{*}\}$ or $\{T_{*} \rightarrow S \rightarrow T^{*}\}$. Also for continuous but arbitrary variations of $X_o(t)$ in time, these control policies and still principal ones to an optimal control policy.

When the entire reactor is on a stationary policy S in time and provided the inlet conversion $X_o(t)$ = constant an optimal operating policy is to maintain the exit conversion $X(1,t)$ = constant.

When the catalyst deactivation is first-order ($m = 1$) then an optimal control policy $\{T^{*}\}$, $\{S \rightarrow T^{*}\}$ or $\{T_{*} \rightarrow S \rightarrow T^{*}\}$ in time is the same everywhere in the reactor.

For $p = 1$, the possibility of an optimal singular control sub-policy existing is noted and conditions under which it may arise are given. An optimal policy in time corresponding to a singular control sub-policy is to maintain the exit conversion $X(1,t)$ = constant. When conditions pertaining to the existence of a singular control sub-policy to an optimal control policy are not satisfied optimal controls defined in τ may only consist of controls T^{*} and T_{*}. For a zero-order reaction the optimal temperature is purely T^{*} everywhere in τ.

For $1 < p < \infty$ no stationary control policy S is an admissible part to an optimal control policy. Therefore an optimal control surface $\hat{T}(z,t)$ defined in may only consist of controls T^{*} and T_{*}, and for a zero-order reaction it is purely T^{*} everywhere.

Since at any given time parts of the bed may have a temperature T^{*} and others T_{*} it is shown that jumps in control in time from a temperature T^{*} to T_{*}

(or vice-versa) over finite lengths of the reactor are not optimal. Therefore in time an optimal temperature change from T^* to T_* or inversely along the length of the reactor bed may only be continuous. Necessary and sufficient conditions defining an extremal control switching line in τ are also given.

The effect of the kinetic parameters n and m on the resulting extremal control policy have been studied and a * assessment of these control policies over more conservative best isothermal policies is given. It is shown that a significant improvement in the total amount of reaction produced, using the extremal distributed control policies, could be expected for low order catalyst deactivation processes with $o < p < \infty$ and high order reaction systems for $p > 1$.

7.1. Future Work

Since the theory presented in chapter 4 allows the treatment of more complex systems the following extensions to the present analytical study could be done,

1. the case where the rate of decay is some function of the reactant and/or product concentration.
2. the case where the rate of reaction is of a more complex nature due to the consideration of a different reaction scheme.
3. the case of an unsteady-state catalytic reaction-deactivation system.

* numerical

LIST OF SYMBOLS

$\bar{a}$	equation (5-96).
$a^{o}_{j}(z,t,\phi^{o},u^{o})$	j^{th} component of a n^{o}-component vector function, equation (2-1).
$a'_{i}(z,t,u)$	i^{th} component of a n'-component vector function, equation (2-2).
$a_{ij}(z,t,\phi,u)$	i^{th} row and j^{th} column element of a n' x n'matrix of coefficients, equation (4-2).
$a'_{ij}(z,t,u^{o})$	i^{th} row and j^{th} column element of a n' x n^{o} matrix of coefficients, equation (2-4).
$a''_{ij}(z,t,\phi)$	i^{th} row and j^{th} column element of a n' x n' matrix of coefficients, equation (2-3).
A	constant defined by equation (3-38).
$\bar{b}$	equation (5-96).
BSTR	ideal batch stirred tank reactor.
$\bar{c}$	equation (5-96).
c_{i}	molar concentration of species i, equation (3-1).
CSTR	ideal continuous stirred tank reactor.
C_{i}	constants, equations (6-4) to (6-6) with i=1,...,5.
C^{*}	constraint control policy characterized by condition (5-17).
C_{*}	constraint control policy characterized by condition (5-18).
$C^{+},C^{+}(z,t)$	optimal control policy in τ.
C_{1}	basic computational algorithm when p > 1 and m $\neq$ 1.
C_{2}	computational algorithm when p > 1 and m = 1.
E_{c}	catalyst deactivation energy.
E_{R}	reaction activation energy.
E_{1}	measure of error relating two successive control switching lines, equation (6-12) of algorithm C_{1}.

E_2^{ℓ}	measure of error at iteration ℓ, equation (6-13) of algorithm C2.
E_3	measure of error relating two successive sets of t_i^*, equation (6-15) of algorithm S1.
E_4	measure of error, equation (6-17) of algorithm S1.
$\bar{f}$	equation (5-96).
$f^0(\underset{\sim}{z},t,\phi^0,\underset{\sim}{u}^0)$	scalar function of equation (2-1).
$f_i(z,t,\underset{\sim}{\phi},\underset{\sim}{u})$	i^{th} component of vector function $\underset{\sim}{f}$.
$\underset{\sim}{f},\underset{\sim}{f}(z,t,\underset{\sim}{\phi},\underset{\sim}{u})$	n'-component vector function, equations (2-2), (2-3) and (4-2).
$f_i'(\underset{\sim}{z},t,\underset{\sim}{\phi}',\underset{\sim}{u}^0)$	i^{th} component of a n'-component vector function, equation (2-4).
f[X]	continuous, generally non-linear, monotonic increasing or decreasing function, or a constant, of conversion X.
F,F[X]	continuous, generally non-linear, monotonic decreasing function, or a constant, of conversion X satisfying relation (3-12).
F'[X]	first derivative of F[X] with respect to X, equation (5-4).
F_1,$F_1(t)$	equation (5-54).
F_1^0	$F_1(t^0)$.
$\bar{g}$	equation (5-96).
g, g[ψ]	continuous, generally non-linear, monotonic increasing function, or a constant, of activity ψ satisfying relation (3-24).
g'[ψ]	first derivative of g[ψ] with respect to ψ, equation (5-5).
$g_i(z,t,\underset{\sim}{\phi},\underset{\sim}{u}^n)$	i^{th} component of a n'-component vector function, equation (4-31).
G_1, G_2', G_2'', G_3	specified scalar functions of functional (4-10).
G_1' $(\underset{\sim}{\phi},\underset{\sim}{u}^n)$	scalar function of equation (4-32).
$h_{ik}(z,t,\underset{\sim}{\phi},\underset{\sim}{u}^n)$	i^{th} row and j^{th} column element of a n' x m matrix of coefficients, equation (4-31).

$H(z,t,\underset{\sim}{\phi},\underset{\sim}{u}^n)$	Hamiltonian like scalar function, equation (4-11).
$H(X,\psi,\lambda,\mu)$	scalar function $H(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u})$ for the problem considered, equation (5-1).
H, $H(z,t)$	particular forms of $H(X,\psi,\lambda,\mu)$ for $p < 1$: equation (5-9), $p = 1$: equation (5-182) or $p > 1$: equation (5-104).
$\bar{H}$, $\bar{H}(z,t)$	scalar function, equation (5-105).
$H'_k(\underset{\sim}{\phi},\underset{\sim}{u}^n)$	k^{th} component of a m-component vector function, equation (4-32).
i	chemical reacting species in system (3-1).
iff	if and only if.
I	functional (4-10).
I_ℓ	ℓ^{th} characteristic line: z = constant, figure 6-1.
II_ℓ	ℓ^{th} characteristic line: t = constant, figure 6-1.
J	total amount of reaction produced over a fixed reaction time with a control k(z,t), equation (3-41).
J^+	value of J obtained with the optimal control $k^+(z,t)$.
J_i	molar flux of species i relative to the molar average velocity v.
J_I	value of J obtained with the best isothermal control policy.
$\bar{J}$	equation (5-96).
k, k[T]	catalyst deactivation rate constant of the Arrhenius form taken as control, equation (3-29).
k*	value of k[T] corresponding to T = T*.
k_*	value of k[T] corresponding to $T = T_*$.
$k(z_i,o)_{new}$	current computed value of $k(z_i,o)$ in step 16 of algorithm S1.
$k(z_i,o)_{old}$	prior computed or assumed value of $k(z_i,o)$, algorithm S1.
k_o	pre-exponential term in equation (3-21).
$k_o(0)$	control k at start-up of the process but uniform along the reactor bed.

$k_o(0)_{new}$	current computed value of $k_o(0)$ in step 16 of algorithm S2.
$k_o(0)_{old}$	prior computed or assumed value of $k_o(0)$, algorithm S2.
$k'[T]$	catalyst deactivation rate constant, equation (3-21).
$\bar{k}$, $\bar{k}(z,t)$	admissible extremal control candidate.
$\hat{k}$, $\hat{k}(z,t)$	extremal control, extremal deactivation rate constant.
k^+, $k^+(z,t)$	optimal control, optimal deactivation rate constant.
K, K[T]	reaction rate constant of the Arrhenius form, equation (3-28).
K^*	value of K[T] correspond to $T = T^*$.
K_*	value of K[T] corresponding to $T = T_*$.
K_o	reaction frequency factor, equation (3-10).
$^oK.$	degree Kelvin.
$K^o(z)$	$K(z,t^o)$.
K'[T]	reaction rate constant of the Arrhenius form, equation (3-10).
$\bar{K}$, $\bar{K}(z,t)$	value of K[T] corresponding to control $\bar{k}$, equation (3-37).
$\hat{K}$, $\hat{K}(z,t)$	value of K[T] corresponding to extremal control $\hat{k}$, equation (3-37).
K^+, $K^+(z,t)$	value of K[T] corresponding to optimal control k^+, equation (3-37).
L	length of the reactor bed.
m, m_j	catalyst deactivation order, equation (3-20); j = 1,...,4, figure 6-8 and equation (6-20).
M	number of characteristic lines II, figure 6-1.
n	order of an irreversible chemical reaction.
$n^{\bullet}$	number of spatial co-ordinates, equation (2-1).
n'	number of dependent variables Φ_i, Φ_i'.
N	number of characteristic lines I, figure 6-1.

p	ratio of E_R/E_c.
PFTR	ideal plug flow tubular reactor.
$P[\eta_1, \eta_2]$	functional expressing the fact that a variation in $X(z,t)$ has the same sign as a variation of parameter η_1 or parameter η_2.
Q(t)	equation (5-171).
r	number of components of control vector $\underset{\sim}{u}$, relation (4-4).
R	ideal gas constant.
R_i	molar rate of production of species i.
$\bar{R}$	equation (5-96).
S	stationary control policy characterized by condition (5-15).
Sg	singular control policy characterized by condition (5-192).
S1	basic computational algorithm when $p < 1$ and $m \neq 1$.
S2	modification of algorithm S1 for $m = 1$.
t	dimensionless time co-ordinate, equation (3-27).
t'	time co-ordinate.
t*	time at which an optimal control policy joins a policy C*.
t_*	time at which an optimal control policy joins a policy C_*.
$t_c, t_j, t_s, t_{sw}, t^o$	reference times.
t_o	specified fixed initial or start-up time.
t_Θ	time required to process one void reactor volume
t_f	specified terminal reaction time.
t_{si}	time at which $\Delta H(z_i, t_{si})$ first reaches a value zero from $t = 1$, algorithm C1.
$(t_{si})_{new}$	current value of t_{si}.
$(t_{si})_{old}$	prior determined or assumed value of t_{si}.
$t_{\bar{s}}$	time $t < t_s$ as defined by equation (5-32).
$t_{\bar{c}}$	time $t < t_c$ with the meaning of equation (5-32).

t_i^o	time at which $\frac{\partial H}{\partial k}$ first reaches a value zero from t = 1, algorithm S1.
t_i^+	arithmetic mean of t_i^* and t_i^o, equation (6-16).
t_i^*	time at which the control $k(z_i,t)$ reaches the value k*, algorithm S1.
$(t_i^*)_{new}$	current value of t_i^*.
$(t_i^*)_{old}$	prior determined value of t_i^*.
t_{min}	lower bound of the set of all t_i^*, algorithm S1.
t_{max}	upper bound of the set of all t_i^*, algorithm S1.
t_c^ℓ	time at which the control switching line intercepts the line z = 0 at iteration ℓ, algorithm C2.
t_H^ℓ	time at which $\Delta H(z,t_H^\ell)$ first reaches a zero value from t = 1 at iteration ℓ, algorithm C2.
T, T(z,t)	temperature (control).
T*	upper bound of permitted temperature T.
T_*	lower bound of temperature T considered.
T_o	uniform starting temperature along the reactor bed, figure 6-5.
T_1, T_2	temperature level.
T^o	total reacting time period, table 5-1.
u_k	k^{th} component of control vector $\underset{\sim}{u}$.
$\underset{\sim}{u}$, $\underset{\sim}{u}(z,t)$	r-component control vector, relation (4-4).
u_i^*, u_{i_*}	i^{th} component of control vector $\underset{\sim}{u}^*$, $\underset{\sim}{u}_*$.
$\underset{\sim}{u}^*$, $\underset{\sim}{u}_*$	r-component upper, lower bound control vector.
$\hat{u}_i$	i^{th} component of the extremal control vector $\underset{\sim}{\hat{u}}$.
$\underset{\sim}{\hat{u}}$, $\underset{\sim}{\hat{u}}(z,t)$	r-component extremal control vector function.
$\underset{\sim}{\bar{u}}$, $\underset{\sim}{\bar{u}}(z,t)$	r-component admissible extremal control vector candidate.
u_K^+	k^{th} component of optimal control vector $\underset{\sim}{u}^+$.
$\underset{\sim}{u}^+$, $\underset{\sim}{u}^+(z,t)$	r-component optimal control vector, relation (4-5).

$\underset{\sim}{u}^{o}$, $\underset{\sim}{u}^{o}(z,t)$	r-component vector function, equations (2-1) and (2-4).
$\underset{\sim}{u}^{\ell}$	control vector defined in relation (4-33).
$\underset{\sim}{u}^{n}$	control vector defined in relation (4-34).
U	closed set of all control vectors $\underset{\sim}{u}$.
$\hat{U}$, $\hat{U}(z,t)$	closed set of all extremal control vectors $\underset{\sim}{\hat{u}}$.
v	molar average velocity, equation (3-1).
$w\ (z,t_{sw})$	control switching line traced out in τ.
X, $X(z,t)$	conversion of an irreversible chemical reaction satisfying relation (3-11).
X_o, $X_o(t)$	inlet conversion to the reactor in time.
$X_1(z')$	conversion along the reactor bed at the start of the process.
X_*	specified lower bound on conversion X.
X_1^*	maximum level of conversion achievable with fresh catalyst $\psi = 1$ and $T = T^*$.
z	dimensionless spatial co-ordinate, equation (3-26).
z'	spatial co-ordinate, independent variable.
z'_j	j^{th} component of vector $\underset{\sim}{z}$.
$\underset{\sim}{z}$	n^o-component vector of spatial co-ordinates, equations (2-1) and (2-4).
z_o	specified distance along the z-axis referring to the beginning of the reactor bed.
z_f	specified distance along the z-axis referring to the end of the reactor bed.
z_i, z_s	reference stations in the reactor, i=1,...,3.
$\bar{z}$	reference stations in the reactor but $\bar{z} \neq z_s$.
$\hat{z}$	stations for which the condition (5-155) holds at time t_s.
z_{sj}^{ℓ}	position along the z-axis at iteration ℓ, algorithm C2.
Z^o	total length of the bed considered, table 5-1.

α	$p/(1-p)$
α_i	i^{th} component of n'-component vector $\underset{\sim}{\alpha}$, equation (4-8).
β	equation (5-72)
β_i	i^{th} component of n'-component vector $\underset{\sim}{\beta}$, equation (4-9).
$\Gamma_k(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},u^n)$	k^{th} component of the n'-component vector function Γ, equation (4-38).
Γ_1, $\Gamma_1(z,t)$	switching function, equation (5-181).
δt, δt_s, δt_i	finite interval of time.
δu_i	i^{th} component of control vector variations $\underset{\sim}{\delta u}$.
$\underset{\sim}{\delta u}$	infinitesimal admissible variations of control vector $\underset{\sim}{u}$, relation (4-23).
δz	finite length of the reactor with $\delta z \subseteq \Delta z$.
δz_o	length of the bed on a control policy S.
δz_1	length of the bed on a control policy C*.
δz_2, $\delta z_2'$, $\delta z_2''$	length of the bed on a control policy C_*.
$\delta\psi$	change in relative catalyst activity in a period of time equal to t_θ.
$\delta\tau^o$	subset of τ whose measure is zero.
$\delta\tau_1$	non-empty open subset $\varepsilon\ \Delta\ \tau_1$.
ΔH	equations (5-13) and (5-107).
Δk	finite admissible variation of k, equations (5-14) and (5-109).
ΔK	equation (5-108).
$\Delta(Kk)$	equation (5-116).
Δt	finite interval of time.
$\underset{\sim}{\Delta u}$	finite admissible variations of control vector $\underset{\sim}{u}$, relation (4-21).
Δz	finite length of the bed.

$\Delta\tau$	non-empty subset of τ.
$\Delta\tau_1$	union of subsets $\delta\tau_1$.
$\Delta\tau_2$	subset of τ defined by relation (4-41).
$\Theta[(\delta\underset{\sim}{u})^3]$	third-order variations of $\delta\underset{\sim}{u}$, equations (4-24) and (4-26).
$\lambda, \lambda(z,t)$	costate variable, equation (5-2).
$\Lambda(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^n)$	scalar function, equation (4-37).
$\mu, \mu(z,t)$	costate variable, equation (5-3).
τ	plane of the independent variables z and t defined by the cartesian product $Z^o \times T^o$.
$\phi, \phi[T,\psi,X]$	rate of catalyst deactivation, equation (3-32).
Φ_i, $\Phi_i(z,t)$	i^{th} component of state vector $\underset{\sim}{\Phi}$.
$\underset{\sim}{\Phi}$, $\underset{\sim}{\Phi}(z,t)$	n'-component state vector, equations (2-2), (2-3) and (4-2).
$\underset{\sim}{\Phi}^+$, $\underset{\sim}{\Phi}^+(z,t)$	optimal state vector $\underset{\sim}{\Phi}$.
Φ^o, $\Phi^o(\underset{\sim}{z},t)$	dependent variable in equation (2-1).
Φ_i', $\Phi_i'(\underset{\sim}{z},t)$	i^{th} component of a n'-component vector $\underset{\sim}{\Phi}'$, equation (2-4).
ψ, $\psi(z,t)$	relative catalyst activity defined by equation (3-13) and satisfying relation (3-23).
ψ_i, $\psi_i(z,t)$	i^{th} component of the n'-component costate vector $\underset{\sim}{\psi}$, equation (4-12).
$\underset{\sim}{\psi}^+$, $\underset{\sim}{\psi}^+(z,t)$	optimal costate vector $\underset{\sim}{\psi}$, equation (4-12).
ψ_o, $\psi_o(z)$	initial relative catalyst activity profile along the reactor length.
$\psi^o(z)$	$\psi(z,t^o)$.
$\bar{\psi}_i$	magnitude of relative catalyst activities corresponding to deactivation order m_i.
ψ_{mean}	average catalyst activity, equation (6-23).
$\Psi_1(z)$	piecewise continuous function of z, or a constant, equation (5-83).
$\Psi_2(t)$	continuous function of t, or a constant, equation (5-83).

Ω, $\Omega[T,\psi,X]$	pseudo-homogeneous rate of reaction, equation (3-8).
∂U	boundary of the set of admissible control vectors U.

MATHEMATICAL SYMBOLS AND OPERATORS

$x = y$	x equal to y.
$x \neq y$	x not equal to y.
$x > y$	x greater than y.
$x \geqslant y$	x greater than or equal to y.
$x < y$	x smaller than y.
$x \leqslant y$	x smaller or equal to y.
$x \varepsilon X$	element x belongs to set X.
$x \notin X$	element x does not belong to set X.
$X \subset Y$	set X is a subset of set Y.
$X \subseteq Y$	set X is a subset of or equal to set Y.
$X \setminus Y$	set X minus set Y.
A => B	fact A implies fact B.
$x \alpha y$	x varies as y.
∞	infinity.
Σ	summation operator.
∇	gradient operator.
dy/dx	derivative of y with respect to x.
$\partial^n y / \partial x^n$	n^{th} partial derivative of y with respect to x.
$\int_{\delta x}$	integral along a path δx.
$\int_x^y$	integral between the limit x and y.

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APPENDIX A

Existence and Uniqueness of a Solution for Systems of First-Order Partial Differential Equations

Consider the following system of first-order partial differential equations:

$$\frac{\partial \Phi_i(z,t)}{\partial t} + \sum_{j=1}^{n} a_{ij}(z,t,\underset{\sim}{\Phi}) \frac{\partial \Phi_j(z,t)}{\partial z} = f_i(z,t,\underset{\sim}{\Phi}) \quad i=1, \ldots,n \tag{A-1}$$

with the associated initial and boundary conditions:

$$\Phi_i(z,t_o) = \alpha_i(z) \qquad i=1,\ldots,n \tag{A-2}$$

$$\Phi_i(z_o,t) = \beta_i(t) \qquad i=1,\ldots,n \tag{A-3}$$

The $\Phi_i(z,t)$ represents the i^{th} component of the unknown n-dimensional vector $\underset{\sim}{\Phi}(z,t)$ distributed in the plane of the independent variables z and t.

The $a_{ij}(z,t,\underset{\sim}{\Phi})$ represents the i^{th} row and j^{th} column element of the n x n matrix $\underline{\underline{A}}(z,t,\underset{\sim}{\Phi})$ and the $f_i(z,t,\underset{\sim}{\Phi})$ corresponds to the i^{th} component of the n-dimensional vector $\underset{\sim}{f}(z,t,\underset{\sim}{\Phi})$.

Generally matrix $\underline{\underline{A}}$ and vector $\underset{\sim}{f}$ may be both function of the variable quantities z, t and $\underset{\sim}{\Phi}$ but not of the partial derivatives of $\underset{\sim}{\Phi}$, that is $\underset{\sim}{\Phi}_z$ or $\underset{\sim}{\Phi}_t$.

When $\underline{\underline{A}}$ does not depend on $\underset{\sim}{\Phi}$ and $\underset{\sim}{f}$ depends linearly on $\underset{\sim}{\Phi}$ the system is linear. If $\underline{\underline{A}}$ is independent of $\underset{\sim}{\Phi}$ and $\underset{\sim}{f}$ depends on $\underset{\sim}{\Phi}$, but non-linearly, the system is called semi-linear and can be treated almost as a linear system. Otherwise, if $\underline{\underline{A}}$ depends on $\underset{\sim}{\Phi}$ the system is termed quasi-linear.

A.1 Analyticity and the Cauchy-Kowalevski Theorem

System (A-1) can be easily expressed in the format of the classical Cauchy problem, which consists in finding the solution of the following system:

$$\frac{\partial \Phi_i(z,t)}{\partial t} = F_i\,(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Phi}_z) \qquad i=1,\ldots,n \tag{A-4}$$

that satisfies the initial conditions (A-2).

The fundamental theorem of Cauchy-Kowalevski then states [Petrovskii (1967)]:

> "If all of the components F_i are analytic functions in some neighbourhood of the point $(z_o,t_o,\underset{\sim}{\Phi}(z_o,t_o))$ and all the components Φ_i and Φ_{z_i} of the column vectors $\underset{\sim}{\Phi}$ and $\underset{\sim}{\Phi}_z$ are analytic functions in some neighbourhood of the point (z_o,t_o), then the Cauchy problem has an analytic solution in some neighbourhood of the point (z_o,t_o) and this solution is unique in the class of analytic functions".

Despite its generality this theorem is restricted to problems involving only analytic functions, that is equations and solutions that have convergent power series representations.

This assumption of analyticity may be regarded in many cases as being not too serious for it is known by the Weierstrass approximation

theorem [Bartle (1964)] that any continuous function can be approximated arbitrarily closely by analytic functions, in fact by polynomials.

This requirement of analyticity may however prove to be very restrictive and to exclude many of the most significant situations in the theory of partial differential equations since the Weierstrass approximation theorem does not insure that close approximation of the boundary values implies close approximation of the solution for $t > t_0$ [Petrovskii (1967), Garabedian (1964)].

A.2 Continuity and the Concept of Characteristics

Nevertheless, for partial differential equations of first-order such as defined by system (A-1) a more direct and complete theory of integration is available under rather weak assumptions of continuity and differentiability.

The key to the theory is the concept of characteristics or the equivalence of a first-order partial differential equation with a certain system of ordinary differential equations.

The basic rationale underlying the use of characteristics is that by an appropriate choice of coordinates the original system can be replaced by an equivalent one expressed in characteristic coordinates.

In terms of these characteristic coordinates differentiation is much simplified since the complication of having more than one differential operator in each equation is removed and the theory is brought closer to that of ordinary differential equations.

The existence and uniqueness of the required solution of the equivalent system then follow directly from the theory of ordinary differential

equations.

A.3 Reduction of Semi-Linear and Linear Systems to a Canonical Form

Reduction of semi-linear or linear systems such as (A-1), involving differentiation in two distinct directions, to a canonical form involving differentiation in a single direction succeeds if and only if such systems are hyperbolic.

This hyperbolicity condition will be stressed here for the more general semi-linear case.

It is immaterial whether the $f_i(z,t,\underset{\sim}{\phi})$ are linear or non-linear functions of the unknown vector $\underset{\sim}{\phi}$, the only assumption will be that the coefficients $a_{ij}(z,t)$ are real and continuous functions of z and t and also that they have continuous partial derivatives with respect to z and t in some region τ of the z,t plane.

In a neighbourhood N(P) of an arbitrarily chosen point $P(z,t) \in \tau$, form n independent linear combinations:

$$\sum_{i=1}^{n} k_{si} \frac{\partial \Phi_i}{\partial t} + \sum_{i=1}^{n} \sum_{j=1}^{n} k_{si}\, a_{ij} \frac{\partial \Phi_j}{\partial z} = \sum_{i=1}^{n} k_{si}\, f_i \qquad s=1,\ldots,n \tag{A-5}$$

of the n equations of system (A-1) such that for all Φ_i $i=1,\ldots,n$:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} k_{si}\, a_{ij}\, \Phi_j = \lambda_s \sum_{i=1}^{n} k_{si}\, \Phi_i \qquad s=1,\ldots,n \tag{A-6}$$

where the $k_{si}(z,t)$ and $\lambda_s(z,t)$ are certain functions with respect to z and t to be more precisely identified later.

It is sufficient and clearly necessary that the coefficients of Φ_j on the two sides of this identity be the same if (A-6) is to hold for all Φ_j in the neighbourhood N(P) of the point $P(z,t) \in \tau$, that is,

$$\sum_{i=1}^{n} k_{si}\, a_{ij} = \lambda_s\, k_{sj} \qquad s=1,\ldots,n \tag{A-7}$$

which is a system of n homogeneous equations for the n unknowns $k_{sj}(z,t)$ $j=1,\ldots,n$.

For this system to have a non-trivial solution, it is necessary and sufficient that the determinant of its coefficients be equal to zero, or,

$$\left| \underline{\underline{A}} - \lambda_s \underline{\underline{I}} \right| = 0 \qquad s=1,\ldots,n \tag{A.8}$$

where $\underline{\underline{I}}$ stands for the n x n identity matrix.

It has been shown [Petrovskii (1967)] that a full set of <u>linearly independent</u> characteristic vectors $k_{sj}(z,t)$ $j=1,\ldots,n$, corresponding to characteristic roots $\lambda_s(z,t)$ is <u>uniquely</u> determined in a neighbourhood N(P) of the point $P(z,t) \in \tau$ if polynomial equation (A-8) has only <u>distinct</u> real characteristic roots in that neighbourhood.

When this last condition is met for the entire region τ under consideration, semi-linear system (A-1) is called <u>totally hyperbolic</u> in the whole of τ and the characteristic roots $\lambda_s(z,t)$ and vectors k_{sj} $j=1,\ldots,n$ have at any point $(z,t) \in \tau$ the same smoothness as the coefficient $a_{ij}(z,t)$ have in τ, that is, they have as many continuous derivatives with respect to

z and t as do the coefficients $a_{ij}(z,t)$.

Under the same hyperbolicity condition, it has also been proven [Petrovskii (1967)] that there exists a non-singular linear transformation of the unknown functions $\underset{\sim}{\phi}(z,t)$ holding for the entire region τ,

$$\epsilon_i(z,t) = \sum_{j=1}^{n} k_{ij}(z,t) \cdot \Phi_j(z,t) \qquad i=1,\ldots,n \tag{A-9}$$

such that semi-linear system (A-1) is reduced to a canonical form.

This can be observed in the following, since the results of (A-5) may be written as:

$$\frac{\partial\{\sum_{i=1}^{n} k_{si}\,\Phi_i\}}{\partial t} + \sum_{j=1}^{n} \frac{\partial\{\sum_{i=1}^{n} k_{si}\,a_{ij}\}\cdot\Phi_j}{\partial z} = f'_s \qquad s=1,\ldots,n \tag{A-10}$$

with

$$f'_s = \sum_{i=1}^{n} k_{si}\,f_i + \sum_{i=1}^{n} \Phi_i \frac{\partial k_{si}}{\partial t} + \sum_{j=1}^{n} \Phi_j \frac{\partial\{\sum_{i=1}^{n} k_{si}\,a_{ij}\}}{\partial z} \qquad s=1,\ldots,n \tag{A-11}$$

Also, using equation (A-7),

$$\frac{\partial\{\sum_{i=1}^{n} k_{si}\,\Phi_i\}}{\partial t} + \frac{\partial\,\lambda_s\{\sum_{j=1}^{n} k_{sj}\,\Phi_j\}}{\partial z} = f'_s \qquad s=1,\ldots,n \tag{A-12}$$

with

$$f'_s = \sum_{i=1}^{n} k_{si} f_i + \sum_{i=1}^{n} \Phi_i \frac{\partial k_{si}}{\partial t} + \sum_{j=1}^{n} \Phi_j \frac{\partial \{\lambda_s k_{sj}\}}{\partial z} \qquad s=1,\ldots,n \qquad \text{(A-13)}$$

Finally in regard to transformations (A-9),

$$\frac{\partial \varepsilon_s}{\partial t} + \lambda_s \frac{\partial \varepsilon_s}{\partial z} = f^*_s \qquad s=1,\ldots,n \qquad \text{(A-14)}$$

with

$$f^*_s = \sum_{i=1}^{n} k_{si} f_i + \sum_{i=1}^{n} \Phi_i \frac{\partial k_{si}}{\partial t} + \lambda_s \sum_{j=1}^{n} \Phi_j \frac{\partial k_{sj}}{\partial z} \qquad s=1,\ldots,n \qquad \text{(A-15)}$$

where f^* is a n-dimensional vector not depending upon any partial derivative of $\underset{\sim}{\varepsilon}$.

The corresponding initial and boundary conditions for system (A-14) are,

$$\varepsilon_s(z,t_o) = \sum_{i=1}^{n} k_{si}(z,t_o) \cdot \alpha_s(z) \qquad s=1,\ldots,n \qquad \text{(A-16)}$$

and

$$\varepsilon_s(z_o,t) = \sum_{i=1}^{n} k_{si}(z_o,t) \cdot \beta_s(t) \qquad s=1,\ldots,n \qquad \text{(A-17)}$$

and are related to conditons (A-2) and (A-3) through transformations (A-9).

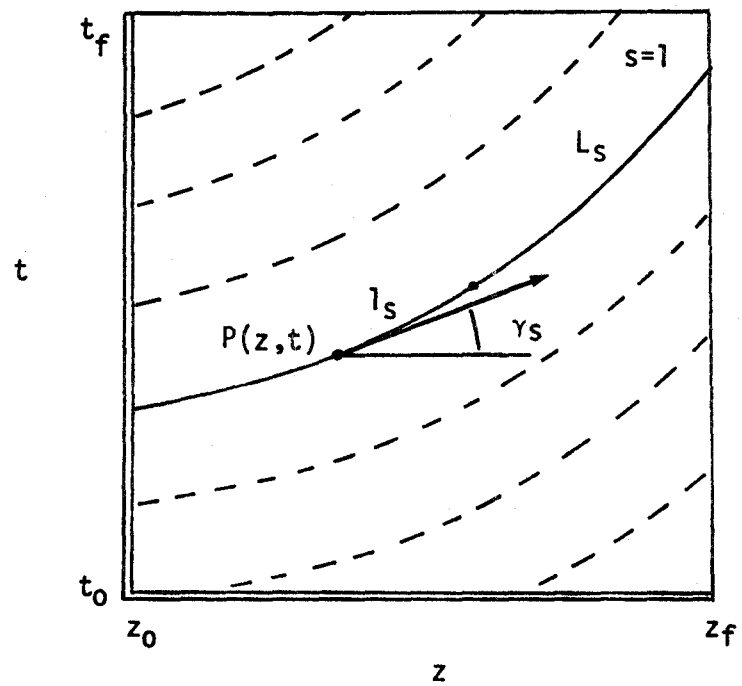
The advantage of the equivalent canonical form (A-14) of semi-linear system (A-1) is that the s^{th} scalar equation of (A-14) can be solved for the derivative of the s^{th} unknown component ε_s of $\underset{\sim}{\varepsilon}$ in the direction of the corresponding characteristic curve L_s defined as,

$$\frac{dz}{dt} = \lambda_s(z,t) \qquad s=1,\ldots,n \tag{A-18}$$

These n equations are called the characteristic lines of system (A-14) for their direction of any point $P(z,t) \in \tau$ is precisely the characteristic direction there.

When semi-linear (A-1) is <u>totally hyperbolic</u> throughout the entire region τ in question, then through every point $(z,t) \in \tau$ there pass a family of n distinct, real characteristic lines L_s $s=1,\ldots,n$.

The figure below represents such a family for a characteristic line L_1.



These characteristic lines originate on the initial-value curve "C" which is determined by the initial and boundary conditions (A-16) and (A-17).

The angle between the tangent to the characteristic curve L_s and the z-axis at point $P(z,t) \in \tau$ is denoted by γ_s and the characteristic directions (A-18) become there,

$$\frac{dz}{dt} = \cot \gamma_s = \lambda_s(z,t) \qquad s=1,\ldots,n \tag{A-19}$$

and by construction, one may write,

$$\frac{dt}{d\ell_s} = \sin \gamma_s = \frac{1}{[1 + \lambda_s^2]^{1/2}} \qquad s=1,\ldots,n \tag{A-20}$$

and

$$\frac{dz}{d\ell_s} = \cos \gamma_s = \frac{\lambda_s}{[1 + \lambda_s^2]^{1/2}} \qquad s=1,\ldots,n \tag{A-21}$$

Also the directional derivative of the function $\varepsilon_s(z,t)$ at any point $P(z,t) \in \tau$ of a characteristic line L_s is given by,

$$\frac{d\,\varepsilon_s}{d\ell_s} = \frac{\partial\,\varepsilon_s}{\partial t} \cdot \frac{dt}{d\ell_s} + \frac{\partial\,\varepsilon_s}{\partial z} \cdot \frac{dz}{d\ell_s} \qquad s=1,\ldots,n \tag{A-22}$$

and denotes the differential of the function $\varepsilon_s(z,t)$ as one moves along the arc ℓ_s in the direction of the characteristic line L_s passing at $P(z,t) \in \tau$.

However, since the directional derivatives (A-22) may also be written

$$\frac{d\,\varepsilon_s}{d\,\ell_s} = \sin\gamma_s \cdot \{\frac{\partial\,\varepsilon_s}{\partial t} + \lambda_s \frac{\partial\,\varepsilon_s}{\partial z}\} \qquad s=1,\ldots,n \qquad (A\text{-}23)$$

the bracketed term is easily identifiable with the s^{th} scalar equation of system (A-14) and,

$$\frac{d\,\varepsilon_s}{d\,\ell_s} = \frac{f_s^*}{[1+\lambda_s^2]^{1/2}} \qquad s=1,\ldots,n \qquad (A\text{-}24)$$

From the above, along a segment of the arc ℓ_s in the direction of the characteristic line L_s the system of partial differential equations (A-14) reduces to a system of ordinary differential equations.

The coordinate z and t given in terms of the parametric coordinate ℓ_s are the following for λ_s constant,

$$t = \frac{\ell_s}{[1+\lambda_s^2]^{1/2}} + \ell_s(z',t') \qquad s=1,\ldots,n \qquad (A\text{-}25)$$

$$z = \frac{\ell_s \cdot \lambda_s}{[1+\lambda_s^2]^{1/2}} + \ell_s(z',t') \qquad s=1,\ldots,n \qquad (A\text{-}26)$$

where $z' \in [z_0,z_f]$ and $t' \in [t_0,t_f]$.

When the characteristic lines L_s do not coincide with the initial-value curve "C", a non-singular transformation of coordinate may be done.

Thus the set of partial differential equations (A-14) can be integrated along the characteristic lines L_s as ordinary differential equations (A-24), and, then each point on the parametrized line ℓ_s can be projected back to the z and t coordinate system using relations (A-25) and (A-26).

Due to the invariance of characteristics under point transformation [Courant and Hilbert (1962)] system (A-24) may also be directly transformed to,

$$\frac{d\,\varepsilon_s}{dt} = f_s^* \qquad s=1,\ldots,n \tag{A-27}$$

using transformation (A-20), and each scalar equation of (A-27) represents the differential of the variable $\varepsilon_s(z,t)$ in time t as one moves along an arc segment ℓ_s of the characteristic line L_s.

Another compatible transformation, using relation (A-21) would be,

$$\frac{d\,\varepsilon_s}{dz} = \frac{f_s^*}{\lambda_s} \qquad s=1,\ldots,n \tag{A-28}$$

where each scalar equation of (A-28) represents the differential of the variable $\varepsilon_s(z,t)$ in space z as one moves along an arc segment ℓ_s of the characteristic line L_s.

Denoting by ℓ_s that portion of the corresponding characteristic line L_s between an arbitrary point $P(z,t) \in \tau$ and its intercept (z',t') with the initial-value curve "C" at time t', the s^{th} scalar equation of (A-27) may be integrated along this arc segment ℓ_s from the point (z',t') to the point $P(z,t) \in \tau$, to give a system of integral equations.

$$\varepsilon_s(z,t) = \varepsilon_s(z',t') + \int_{t'}^{t} f_s^* \, d\ell_s \qquad s=1,\ldots,n \qquad \text{(A-29)}$$

Similarly for the s^{th} scalar equation of (A-28),

$$\varepsilon_s(z,t) = \varepsilon_s(z',t') + \int_{z'}^{z} \frac{f_s^*}{\lambda_s} \, d\ell_s \qquad s=1,\ldots,n \qquad \text{(A-30)}$$

where again here $\varepsilon_s(z',t')$ refers to the condition on the initial-value curve "C".

Every solution to system (A-27) or (A-28) that satisfies the initial condition $\varepsilon_s(z',t')$ is a solution of the system of integral equations (A-29) or (A-30) and conversely.

A.4 Hyperbolic Systems and the Cauchy Problem

It is shown in section A.3 that totally hyperbolic system of first-order partial differential equations can be reduced to some suitable canonical form under rather weak assumptions of continuity and differentiability.

The assumption of a totally hyperbolic system for which all of the real characteristic roots $\lambda_i(z,t)$, $i=1,\ldots,n$, are distinct has been shown not to be essential for that reduction to succeed [Petrovskii (1967), Garabedian (1964)].

All the statements made in section A.3 may be shown to remain valid for the case in which some of the real characteristic roots $\lambda_i(z,t)$ coincide

if and only if the resulting set of characteristic vectors $k_{sj}(z,t)$ $j=1,\ldots,n$, generated is linearly independent [Petrovskii (1967)]. When this is the case, the system is called hyperbolic.

Questions about the existence of a solution and uniqueness of that solution for the original Cauchy initial-value problem for the totally hyperbolic system (A-1) with the initial data (A-2) and (A-3) are then essentially transposed to the equivalent system of ordinary differential equations (A-24) with the initial-value curve "C" as initial conditions.

Theory pertaining to a system of ordinary differential equations is fairly complete and general existence and uniqueness theorems are available [Coddington and Levinson (1955)]. Proofs of these theorems are fairly lengthy and intricate.

In the first place, it is necessary to establish the existence of a continuous vector function $\underset{\sim}{\varepsilon}(z,t)$ such that each of its components $\varepsilon_s(z,t) = \varepsilon_s(z',t')$, $s=1,\ldots,n$ on the given initial data curve "C" and satisfied the differential equations (A-24) in a neighbourhood $N(P_0)$ of a point $P_0[z',t', \underset{\sim}{\varepsilon}(z',t')]$.

In order to do this the equivalence of the given initial-value problem with a certain set of integrals is shown.

A sequence of vector functions is constructed in such a manner that the limit vector function of the sequence can be shown to exist, and to satisfy the integral equations; this vector function being also a solution of the initial-value problem. This leads to the Cauchy-Peano existence theorem.

Finally, it is shown that any other solution of the initial-value problem, regardless of its manner of construction, is identical to the first solution. Hence the solution is unique. The Picard-Lindelof theorem summarizes

these arguments.

Conditions under which the existence of a solution to the totally hyperbolic system (A-24) with the initial-data curve "C" will be ascertained by the Cauchy-Peano existence theorem in a neighbourhood $N(P_0)$ of the point $P_0[z',t', \underset{\sim}{\varepsilon}(z',t')]$ is that the vector function $\underset{\sim}{f}^*$ be a <u>continuous function of its arguments</u> there, that is,

$$\boxed{\underset{\sim}{f}^* \in C^0 \text{ in } N(P_0)} \tag{A-31}$$

However, something more than the continuity of the vector function $\underset{\sim}{f}^*$ in $N(P_0)$ is required in order to guarantee that a solution $\underset{\sim}{\varepsilon}(z,t)$ passing through a given point $P[z,t, \underset{\sim}{\varepsilon}(z,t)] \in N(P_0)$ be unique.

A simple condition which permits one to imply uniqueness of a solution through the Picard-Lindelof theorem is that the vector function $\underset{\sim}{f}^*$ satisfies a Lipschitz condition with respect to the unknown vector function $\underset{\sim}{\varepsilon}$ in $N(P_0)$, that is,

$$\boxed{\underset{\sim}{f}^* \in \text{Lip} \text{ in } N(P_0)} \tag{A-32}$$

The precise meaning of that condition may be expressed in the fact that if the vector function $\underset{\sim}{f}^*$ is defined in the space $(z,t,\underset{\sim}{\varepsilon}) \in N(P_0)$ and that there exist a constant $M > 0$ such that for every $(z,t,\underset{\sim}{\varepsilon}^1)$ and $(z,t,\underset{\sim}{\varepsilon}^2)$ in $N(P_0)$.

$$|\underset{\sim}{f}^*(z,t,\underset{\sim}{\varepsilon}^1) - \underset{\sim}{f}^*(z,t,\underset{\sim}{\varepsilon}^2)| \leq M \cdot |\underset{\sim}{\varepsilon}^1 - \underset{\sim}{\varepsilon}^2| \tag{A-33}$$

then the vector function $\underset{\sim}{f}^*$ is said to satisfy a Lipschitz condition with respect to $\underset{\sim}{\varepsilon}$ in $N(P_0)$, and $\underset{\sim}{f}^*$ is uniformly continuous in $\underset{\sim}{\varepsilon}$ for each fixed station (z,t) in $N(P_0)$, although nothing is implied concerning the continuity of $\underset{\sim}{f}^*$ with respect to z and t. The constant M is often called a Lipschitz constant.

Nevertheless, since the existence and uniqueness theorems of such a general nature can only insure a solution in the small, that is, in some neighbourhood $N(P_0)$ of the whole space $(z,t,\underset{\sim}{\varepsilon})$ when,

$$\boxed{f^* \in \{C^0, \text{Lip}\} \text{ in } N(P_0)} \qquad \text{(A-34)}$$

the existence and uniqueness of a solution $\underset{\sim}{\varepsilon}(z,t)$ in the large can only be asserted under additional conditions on the system coefficients and the initial data.

In general, the existence and uniqueness of a continuous solution $\underset{\sim}{\varepsilon}(z,t)$ with continuous first derivatives with respect to z and t can be extended into the whole space Γ of z,t and $\underset{\sim}{\varepsilon}(z,t)$ under consideration as long as the coefficient $a_{ij}(z,t)$, the vector function $\underset{\sim}{f}^*$ and the initial data (A-16) and (A-17) of the system retain their continuity and differentiability in that space [Courant and Hilbert (1962), Coddington (1961)].

However, the initial-value problem (A-24) with the initial data curve for which a solution exists and is uniquely determined in the whole of Γ may still be incorrectly set or not well posed [Courant and Hilbert (1962)].

This results from Hadamard's work in the theory of partial differential equations which has shown that a third criterion necessary for a problem of

this type to be correctly set or proper in that sense is that its solution must also depend continuously on the data.

Fortunately, however, a sufficient condition for the system at hand to be proper in the sense of Hadamard has been shown [Courant and Hilbert (1962)] that it be totally hyperbolic in the whole of Γ.

APPENDIX B

PROOF OF A MAXIMUM PRINCIPLE

B.1 Control Perturbation and Functional Increment

The general derivation of the necessary conditions for optimality are based on the following observation.

If there exists an admissible optimal control policy which yields a minimum for the cost functional I, then any different admissible control policy will result in no lower values for the cost functional.

This concept of non-decreasing cost of the functional I for any sub-optimal control policy is then used to derive the necessary conditions for an optimal control to exist.

Noting that the cost functional as defined by (4-10) may be written in terms of the function H defined by (4-11), the increment ΔI corresponding to an arbitrary perturbation in control $\Delta\underset{\sim}{u}(z,t)$ is,

$$\Delta I = \int_{t_o}^{t_f} \int_{z_o}^{z_f} \{- \Delta\bar{H} + \sum_{i=1}^{n} \Delta [\psi_i . f_i]\} \, dz \, dt$$

$$+ \int_{t_o}^{t_f} \{\Delta G_2' [\underset{\sim}{\phi}(z_o,t)] + \Delta G_2'' [\underset{\sim}{\phi}(z_f,t)]\} \, dt \qquad \text{(B-1)}$$

$$+ \int_{z_o}^{z_f} \Delta G_3 [\underset{\sim}{\phi}(z,t_f)] \, dz$$

where

$$\Delta\bar{H} = H(z,t,\underset{\sim}{\phi} + \Delta\underset{\sim}{\phi},\underset{\sim}{\psi} + \Delta\underset{\sim}{\psi},\underset{\sim}{u} + \Delta\underset{\sim}{u}) - H(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}) \tag{B-2}$$

and

$$\sum_{i=1}^{n} \Delta\,[\psi_i . f_i] = \sum_{i=1}^{n} \psi_i . \Delta f_i + \sum_{i=1}^{n} f_i . \Delta\psi_i + \sum_{i=1}^{n} \Delta\psi_i . \Delta f_i \tag{B-3}$$

$$\Delta G_2' \,[\underset{\sim}{\phi}(z_o,t)] = G_2' \,[\underset{\sim}{\phi}(z_o,t) + \Delta\underset{\sim}{\phi}(z_o,t)] - G_2' \,[\underset{\sim}{\phi}(z_o,t)] \tag{B-4}$$

$$\Delta G_2'' \,[\underset{\sim}{\phi}(z_f,t)] = G_2'' \,[\underset{\sim}{\phi}(z_f,t) + \Delta\underset{\sim}{\phi}(z_f,t)] - G_2'' \,[\underset{\sim}{\phi}(z_f,t)] \tag{B-5}$$

$$\Delta G_3 \,[\underset{\sim}{\phi}(z,t_f)] = G_3 \,[\underset{\sim}{\phi}(z,t_f) + \Delta\underset{\sim}{\phi}(z,t_f)] - G_3 \,[\underset{\sim}{\phi}(z,t_f)] \tag{B-6}$$

However since $\underset{\sim}{\phi}(z_o,t)$ is not influenced by a variation of control in τ, $\Delta\underset{\sim}{\phi}(z_o,t) = 0$ and consequently,

$$\int_{t_o}^{t_f} \Delta G_2' [\underset{\sim}{\phi}(z_o,t)]\, dt = 0 \tag{B-7}$$

and the functional increment (B-1) reduces to,

$$\Delta I = \int_{t_o}^{t_f} \int_{z_o}^{z_f} \{-\Delta\bar{H} + \sum_{i=1}^{n} \Delta [\psi_i . f_i]\} \, dz \, dt \qquad (B\text{-}8)$$

$$+ \int_{t_o}^{t_f} \Delta G_2'' [\underset{\sim}{\phi}(z_f,t)] \, dt + \int_{z_o}^{z_f} \Delta G_3 [\underset{\sim}{\phi}(z,t_f)] \, dz$$

$\Delta\bar{H}$ expression

The increment $\Delta\bar{H}$ defined by equation (B-2) may also be written as,

$$\Delta\bar{H} = \Delta\bar{\bar{H}} + \Delta H \qquad (B\text{-}9)$$

where

$$\Delta\bar{\bar{H}} = H(z,t,\underset{\sim}{\phi} + \Delta\underset{\sim}{\phi}, \underset{\sim}{\psi} + \Delta\underset{\sim}{\psi}, \underset{\sim}{u} + \Delta\underset{\sim}{u}) - H(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u}) \qquad (B\text{-}10)$$

and

$$\Delta H = H(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u}) - H(z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}) \qquad (B\text{-}11)$$

Recalling the Mean Value Theorem and Taylor's Theorem for functions of several variables [Bartle (1964)]:

Mean Value Theorem

Let f be defined on a subset Q of R^p and have values in R. Suppose the set Q contains the points a,b and the line segment joining them and that f is differentiable at every point of this segment. Then there exists a point c on this line segment such that,

$$f(b) - f(a) = D\,f(c) \,.\, (b-a) \tag{B-12}$$

Taylor's Theorem

Suppose that f is a function with domain Q in R^p and range in R, and suppose that f has continuous partial derivatives of order n in a neighborhood of every point on a line segment joining two points u,v in Q. Then there exists a point $\bar{u}$ on this line segment such that,

$$f(v) = f(u) + \frac{1}{1!} D\,f(u).(v-u) + \frac{1}{2!} D^2 f(u).(v-u)^2 + \ldots + \frac{1}{n!} D^n f(\bar{u}).(v-u)^n \tag{B-13}$$

and noting that the scalar function H is at least twice continuously differentiable with respect to its augments, expression (B-10) for $\Delta\bar{\bar{H}}$ may then be expanded exactly to second-order terms.

$$\Delta\bar{\bar{H}} = H(z,t,\underset{\sim}{\Phi}+\Delta\underset{\sim}{\Phi},\underset{\sim}{\psi}+\Delta\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u}) - H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u})$$

$$= \sum_{j=1}^{n} \frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u})}{\partial \psi_j}\,\Delta\Phi_j + \sum_{i=1}^{n} \frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u})}{\partial \Phi_i} \,.\, \Delta\Phi_i \quad +$$

$$+\frac{1}{2}\sum_{j=1}^{n}\sum_{i=1}^{n}\frac{\partial^2 H(z,t,\underset{\sim}{\Phi}+\theta^1_{\Phi}\underset{\sim}{\Delta\Phi},\underset{\sim}{\Psi}+\theta^1_{\Psi}\underset{\sim}{\Delta\Psi},\underset{\sim}{u}+\underset{\sim}{\Delta u})}{\partial\Phi_j\,\partial\Phi_i}\cdot\Delta\Phi_i\cdot\Delta\Phi_j$$

$$+\sum_{j=1}^{n}\sum_{i=1}^{n}\frac{\partial^2 H(z,t,\underset{\sim}{\Phi}+\theta^1_{\Phi}\underset{\sim}{\Delta\Phi},\underset{\sim}{\Psi}+\theta^1_{\Psi}\underset{\sim}{\Delta\Psi},\underset{\sim}{u}+\underset{\sim}{\Delta u})}{\partial\Psi_j\,\partial\Phi_i}\cdot\Delta\Phi_i\cdot\Delta\Psi_j \qquad \text{(B-14)}$$

$$+\frac{1}{2}\sum_{j=1}^{n}\sum_{j=1}^{n}\frac{\partial^2 H(z,t,\underset{\sim}{\Phi}+\theta^1_{\Phi}\underset{\sim}{\Delta\Phi},\underset{\sim}{\Psi}+\theta^1_{\Psi}\underset{\sim}{\Delta\Psi},\underset{\sim}{u}+\underset{\sim}{\Delta u})}{\partial\Psi_j\,\partial\Psi_i}\cdot\Delta\Psi_i\cdot\Delta\Psi_j$$

Since ΔH defined by equation (B-11) can also be expanded exactly to first order terms,

$$H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u}+\underset{\sim}{\Delta u}) = H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u}) + \sum_{k=1}^{r}\frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u}+\theta^1_{u}\underset{\sim}{\Delta u})}{\partial u_k}\cdot\Delta u_k \qquad \text{(B-15)}$$

and from equation (B-14) with result (B-15),

$$\sum_{j=1}^{n}\frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u}+\underset{\sim}{\Delta u})}{\partial\Psi_j}\cdot\Delta\Psi_j + \sum_{i=1}^{n}\frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u}+\underset{\sim}{\Delta u})}{\partial\Phi_i}\cdot\Delta\Phi_i$$

$$=\sum_{j=1}^{n}\frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u})}{\partial\Psi_j}\cdot\Delta\Psi_j + \sum_{i=1}^{n}\frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u})}{\partial\Phi_i}\cdot\Delta\Phi_i \qquad \text{(B-16)}$$

$$+\sum_{j=1}^{n}\sum_{k=1}^{r}\frac{\partial^2 H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u}+\theta^1_{u}\underset{\sim}{\Delta u})}{\partial\Psi_j\,\partial u_k}\cdot\Delta u_k\cdot\Delta\Psi_j$$

$$+\sum_{i=1}^{n}\sum_{k=1}^{r}\frac{\partial^2 H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\Psi},\underset{\sim}{u}+\theta^1_{u}\underset{\sim}{\Delta u})}{\partial\Phi_i\,\partial u_k}\cdot\Delta u_k\cdot\Delta\Phi_i$$

Substituting this result in expression (B-14), $\Delta\bar{H}$ may be rewritten,

$$\Delta\bar{H} = \Delta H + \sum_{j=1}^{n} \frac{\partial H}{\partial \psi_j} \cdot \Delta\psi_j + \sum_{i=1}^{n} \frac{\partial H}{\partial \Phi_i} \cdot \Delta\Phi_i + \varepsilon_1 \tag{B-17}$$

with

$$\begin{aligned}
\varepsilon_1 = & \sum_{j=1}^{n} \sum_{k=1}^{r} \frac{\partial^2 H_1}{\partial \psi_j \, \partial u_k} \cdot \Delta u_k \cdot \Delta\psi_j \\
& + \sum_{i=1}^{n} \sum_{k=1}^{r} \frac{\partial^2 H_1}{\partial \Phi_i \, \partial u_k} \cdot \Delta u_k \cdot \Delta\Phi_i \\
& + \frac{1}{2} \sum_{j=1}^{n} \sum_{i=1}^{n} \frac{\partial^2 H_2}{\partial \psi_j \, \partial \Phi_i} \cdot \Delta\Phi_i \cdot \Delta\Phi_j \\
& + \sum_{j=1}^{n} \sum_{i=1}^{n} \frac{\partial^2 H_2}{\partial \psi_j \, \partial \Phi_i} \cdot \Delta\Phi_i \cdot \Delta\psi_j \\
& + \frac{1}{2} \sum_{j=1}^{n} \sum_{i=1}^{n} \frac{\partial^2 H_2}{\partial \psi_j \, \partial \psi_i} \cdot \Delta\psi_i \cdot \Delta\psi_j
\end{aligned} \tag{B-18}$$

where

$$\begin{aligned}
H &= H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},\underset{\sim}{u}) \\
H_1 &= H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},\underset{\sim}{u}+\underset{\sim}{\theta}^1_{u}\Delta\underset{\sim}{u}) \\
H_2 &= H(z,t,\underset{\sim}{\Phi}+\underset{\sim}{\theta}^1_{\Phi}\Delta\underset{\sim}{\Phi},\underset{\sim}{\psi}+\underset{\sim}{\theta}^1_{\psi}\Delta\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u})
\end{aligned} \tag{B-19}$$

and $$0 \leq \underset{\sim}{\theta}^1_{\Phi}, \underset{\sim}{\theta}^1_{\psi}, \underset{\sim}{\theta}^1_{u} \leq 1$$

$\sum_{i=1}^{n} \Delta[\psi_i \cdot f_i]$ expression:

The effect of a control perturbation upon the state variables of the system is carried out through equation (4-2), and,

$$\Delta f_i = \frac{\partial\, \Delta\Phi_i}{\partial t} + \sum_{j=1}^{n} a_{ij} \frac{\partial\, \Delta\Phi_j}{\partial z} \qquad i=1,\ldots,n \tag{B-20}$$

Since from equation (4-11),

$$f_i = \frac{\partial H}{\partial \psi_i} \qquad i=1,\ldots,n \tag{B-21}$$

the increment Δf_i may also be written,

$$\Delta f_i = \Delta \frac{\partial H}{\partial \psi_i} = \frac{\partial H(z,t,\underset{\sim}{\Phi}+\Delta\underset{\sim}{\Phi},\underset{\sim}{\psi}+\Delta\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u})}{\partial \psi_i} - \frac{\partial H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},\underset{\sim}{u})}{\partial \psi_i} \tag{B-22}$$

or recalling equation (B-2),

$$\Delta f_i = \frac{\partial \Delta \bar{H}}{\partial \psi_i} \tag{B-23}$$

Expanding $\Delta\bar{H}$ exactly to first-order terms gives,

$$\begin{aligned}
\Delta \bar{H} &= H(z,t,\underset{\sim}{\Phi}+\Delta\underset{\sim}{\Phi},\underset{\sim}{\psi}+\Delta\underset{\sim}{\psi},\underset{\sim}{u}+\Delta\underset{\sim}{u}) - H(z,t,\underset{\sim}{\Phi},\underset{\sim}{\psi},\underset{\sim}{u}) \\
&= \sum_{i=1}^{n} \frac{\partial H(z,t,\underset{\sim}{\Phi}+\theta^2_{\underset{\sim}{\Phi}\underset{\sim}{\Phi}}\Delta\underset{\sim}{\Phi},\underset{\sim}{\psi}+\theta^2_{\underset{\sim}{\psi}\underset{\sim}{\psi}}\Delta\underset{\sim}{\psi},\underset{\sim}{u}+\theta^2_{\underset{\sim}{u}\underset{\sim}{u}}\Delta\underset{\sim}{u})}{\partial \Phi_i} \cdot \Delta\Phi_i \\
&+ \sum_{j=1}^{n} \frac{\partial H(z,t,\underset{\sim}{\Phi}+\theta^2_{\underset{\sim}{\Phi}\underset{\sim}{\Phi}}\Delta\underset{\sim}{\Phi},\underset{\sim}{\psi}+\theta^2_{\underset{\sim}{\psi}\underset{\sim}{\psi}}\Delta\underset{\sim}{\psi},\underset{\sim}{u}+\theta^2_{\underset{\sim}{u}\underset{\sim}{u}}\Delta\underset{\sim}{u})}{\partial \psi_j} \cdot \Delta\psi_j \\
&+ \sum_{k=1}^{r} \frac{\partial H(z,t,\underset{\sim}{\Phi}+\theta^2_{\underset{\sim}{\Phi}\underset{\sim}{\Phi}}\Delta\underset{\sim}{\Phi},\underset{\sim}{\psi}+\theta^2_{\underset{\sim}{\psi}\underset{\sim}{\psi}}\Delta\underset{\sim}{\psi},\underset{\sim}{u}+\theta^2_{\underset{\sim}{u}\underset{\sim}{u}}\Delta\underset{\sim}{u})}{\partial u_k} \cdot \Delta u_k
\end{aligned} \tag{B-24}$$

Substituting this result in equation (B-23),

$$\Delta f_i = \sum_{j=1}^{n} \frac{\partial^2 H_3}{\partial \psi_i \, \partial \Phi_j} \cdot \Delta \Phi_j + \sum_{j=1}^{n} \frac{\partial^2 H_3}{\partial \psi_i \, \partial \psi_j} \cdot \Delta \psi_j + \sum_{k=1}^{r} \frac{\partial^2 H_3}{\partial \psi_i \, \partial u_k} \cdot \Delta u_k \qquad \text{(B-25)}$$

Thus the third component of equation (B-3) may be written,

$$\sum_{i=1}^{n} \Delta \psi_i \cdot \Delta f_i = \varepsilon_2 \qquad \text{(B-26)}$$

where

$$\varepsilon_2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 H_3}{\partial \psi_i \, \partial \Phi_j} \cdot \Delta \Phi_j \cdot \Delta \psi_i + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 H_3}{\partial \psi_i \, \partial \psi_j} \cdot \Delta \psi_j \cdot \Delta \psi_i + \sum_{i=1}^{n} \sum_{k=1}^{r} \frac{\partial^2 H_3}{\partial \psi_i \, \partial u_k} \cdot \Delta u_k \cdot \Delta \psi_i \qquad \text{(B-27)}$$

with

$$H_3 = H(z, t, \underset{\sim}{\Phi} + \theta^2_{\underset{\sim}{\Phi}} \cdot \underset{\sim}{\Delta \Phi}, \underset{\sim}{\psi} + \theta^2_{\underset{\sim}{\psi}} \underset{\sim}{\Delta \psi}, \underset{\sim}{u} + \theta^2_{\underset{\sim}{u}} \underset{\sim}{\Delta u}) \qquad \text{(B-28)}$$

and $\quad 0 \leq \theta^2_{\underset{\sim}{\Phi}}, \theta^2_{\underset{\sim}{\psi}}, \theta^2_{\underset{\sim}{u}} \leq 1$

Also by equation (B-21) the second component of equation (B-3) becomes,

$$\sum_{i=1}^{n} f_i \cdot \Delta \psi_i = \sum_{i=1}^{n} \frac{\partial H}{\partial \psi_i} \cdot \Delta \psi_i \qquad \text{(B-29)}$$

Equation (B-20) finally permits one to write for the first component of equation (B-3),

$$\sum_{i=1}^{n} \psi_i \cdot \Delta f_i = \sum_{i=1}^{n} \{ \psi_i \frac{\partial \Delta \Phi_i}{\partial t} + \sum_{j=1}^{n} \psi_i \cdot a_{ij} \frac{\partial \Delta \Phi_j}{\partial z} \} \qquad \text{(B-30)}$$

and

$$\sum_{i=1}^{n} \Delta [\psi_i . f_i] = \varepsilon_2 + \sum_{i=1}^{n} \{\frac{\partial H}{\partial \psi_i} . \Delta\psi_i + \psi_i \frac{\partial \Delta\Phi_i}{\partial t} + \sum_{j=1}^{n} \psi_i . a_{ij} \frac{\partial \Delta\Phi_j}{\partial z} \} \qquad \text{(B-31)}$$

Functional Increment ΔI:

Substituting equations (B-17) and (B-31) into (B-8), the functional increment ΔI becomes,

$$\Delta I = - \int_{t_o}^{t_f} \int_{z_o}^{z_f} \Delta H \, dz \, dt + \int_{t_o}^{t_f} \int_{z_o}^{z_f} [\varepsilon_2 - \varepsilon_1] \, dz \, dt$$

$$+ \int_{t_o}^{t_f} \int_{z_o}^{z_f} \sum_{i=1}^{n} \{\psi_i \frac{\partial \Delta\Phi_i}{\partial t} + \sum_{j=1}^{n} \psi_i . a_{ij} \frac{\partial \Delta\Phi_j}{\partial z} - \frac{\partial H}{\partial \Phi_i} . \Delta\Phi_i\} \, dz \, dt \qquad \text{(B-32)}$$

$$+ \int_{t_o}^{t_f} \Delta G_2'' [\underset{\sim}{\Phi}(z_f, t)] \, dt + \int_{z_o}^{z_f} \Delta G_3 [\Phi(z, t_f)] \, dz$$

Recalling equations (4-12), the third integral of equation (B-32) may be written,

$$\int_{t_o}^{t_f} \int_{z_o}^{z_f} \sum_{i=1}^{n} \{\psi_i \frac{\partial \Delta\Phi_i}{\partial t} + \sum_{j=1}^{n} \psi_i . a_{ij} \frac{\partial \Delta\Phi_j}{\partial z} + \Delta\Phi_i \frac{\partial \psi_i}{\partial t} + \sum_{j=1}^{n} \Delta\Phi_i \frac{\partial a_{ij} . \psi_j}{\partial z}\} \, dz \, dt \qquad \text{(B-33)}$$

or grouping,

$$\int_{t_o}^{t_f}\int_{z_o}^{z_f} \sum_{i=1}^{n} \{\frac{\partial[\psi_i . \Delta\Phi_i]}{\partial t} + \sum_{j=1}^{n} \frac{\partial[a_{ij}\psi_i\Delta\Phi_j]}{\partial z}\}\, dz\, dt \qquad \text{(B-34)}$$

Each partial differential term may be individually integrated with respect to its coordinate, and noting that

$$\Delta\underset{\sim}{\phi}(z,t_o) \equiv \Delta\underset{\sim}{\phi}(z_o,t) = 0 \qquad \text{(B-35)}$$

the double integral (B-34) reduces to,

$$\int_{z_o}^{z_f} \sum_{i=1}^{n} \{\psi_i(z,t_f) \,.\, \Delta\Phi_i(z,t_f)\} \,.\, dz$$

$$+ \int_{t_o}^{t_f} \sum_{i=1}^{n}\sum_{j=1}^{n} \{a_{ij}(z_f,t) \,.\, \psi_i(z_f,t) \,.\, \Delta\Phi_j(z_f.t)\} \,.\, dt \qquad \text{(B-36)}$$

However, observing the terminal and boundary conditions (4-13) and (4-14), result (B-36) becomes,

$$-\int_{z_o}^{z_f} \sum_{i=1}^{n} \{\frac{\partial\, G_3[\underset{\sim}{\phi}(z,t_f)]}{\partial\phi_i(z,t_f)} \,.\, \Delta\Phi_i(z,t_f)\} \,.\, dz \qquad +$$

$$- \int_{t_o}^{t_f} \sum_{j=1}^{n} \{ \frac{\partial\, G_2''[\underset{\sim}{\phi}(z_f,t)]}{\partial \Phi_j(z_f,t)} \cdot \Delta\Phi_j(z_f,t) \} \cdot dt \tag{B-37}$$

and functional increment (B-32) is rewritten,

$$\Delta I = - \int_{t_o}^{t_f} \int_{z_o}^{z_f} \Delta H \, dz \, dt + \int_{t_o}^{t_f} \int_{z_o}^{z_f} [\varepsilon_2 - \varepsilon_1] \, dz \, dt$$

$$+ \int_{t_o}^{t_f} \{\Delta\, G_2''[\underset{\sim}{\phi}(z_f,t)] - \sum_{j=1}^{n} \frac{\partial\, G_2''[\phi(z_f,t)]}{\partial \Phi_j(z_f,t)} \cdot \Delta\Phi_j(z_f,t)\} \cdot dt \tag{B-38}$$

$$+ \int_{z_o}^{z_f} \{\Delta\, G_3[\underset{\sim}{\phi}(z,t_f)] - \sum_{i=1}^{n} \frac{\partial\, G_3[\underset{\sim}{\phi}(z,t_f)]}{\partial \Phi_i(z,t_f)} \cdot \Delta\Phi_i(z,t_f)\} \quad dz$$

Since $G_2''[\underset{\sim}{\phi}(z_f,t)]$ and $G_3[\underset{\sim}{\phi}(z,t_f)]$ are twice continuously differentiable functions with respect to their arguments, $\Delta\, G_2''[\phi(z_f,t)]$ and $\Delta\, G_3[\underset{\sim}{\phi}(z,t_f)]$ as defined by equations (B-5) and (B-6) can be expanded exactly to second order terms,

$$\Delta\, G_2''[\underset{\sim}{\phi}(z_f,t)] = \sum_{j=1}^{n} \frac{\partial\, G_2''[\underset{\sim}{\phi}(z_f,t)]}{\partial \Phi_j(z_f,t)} \cdot \Delta\Phi_j(z_f,t) \tag{B-39}$$

$$+ \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2\, G_2''[\underset{\sim}{\phi}(z_f,t) + \underset{\sim}{\theta} G_2'' \Delta\underset{\sim}{\phi}(z_f,t)]}{\partial \Phi_i(z_f,t)\, \partial \Phi_j(z_f,t)} \cdot \Delta\Phi_j(z_f,t) \cdot \Delta\Phi_i(z_f,t)$$

and

$$\Delta G_3[\underset{\sim}{\phi}(z,t_f)] = \sum_{i=1}^{n} \frac{\partial G_3[\underset{\sim}{\phi}(z,t_f)]}{\partial \Phi_i(z,t_f)} \cdot \Delta\Phi_i(z,t_f) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 G_3[\underset{\sim}{\phi}(z,t_f) + \underset{\sim}{\theta} G_3 \Delta\underset{\sim}{\phi}(z,t_f)]}{\partial \Phi_i(z,t_f) \cdot \partial \Phi_j(z,t_f)} \cdot \Delta\Phi_j(z,t_f) \cdot \Delta\Phi_i(z,t_f) \tag{B-40}$$

Substituting these last results in the functional increment (B-38) gives finally,

$$\Delta I = - \int_{t_o}^{t_f} \int_{z_o}^{z_f} \Delta H \, dz \, dt + \beta \tag{B-41}$$

where the remainder term β is given by

$$\beta = \int_{t_o}^{t_f} \int_{z_o}^{z_f} [\varepsilon_2 - \varepsilon_1] \, dz \, dt + \frac{1}{2} \int_{t_o}^{t_f} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 G''_{2_a}}{\partial \Phi_i(z_f,t) \, \partial \Phi_j(z_f,t)} \cdot \Delta\Phi_j(z_f,t) \cdot \Delta\Phi_i(z_f,t) \, dt + \frac{1}{2} \int_{z_o}^{z_f} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 G_{3_a}}{\partial \Phi_i(z,t_f) \, \partial \Phi_j(z,t_f)} \cdot \Delta\Phi_j(z,t_f) \cdot \Delta\Phi_i(z,t_f) \, dz \tag{B-42}$$

and,

$$G''_{2_a} = G''_2 \left[\underset{\sim}{\phi}(z_f,t) + \underset{\sim}{\theta}_{G''_2}\underset{\sim}{\Delta\phi}(z_f,t)\right]$$

$$G_{3_a} = G_3 \left[\underset{\sim}{\phi}(z,t_f) + \underset{\sim}{\theta}_{G_3}\underset{\sim}{\Delta}(z,t_f)\right] \qquad \text{(B-43)}$$

with $\quad 0 \leq \underset{\sim}{\theta}_{G''_2}, \underset{\sim}{\theta}_{G_3} \leq 1$

Expressions (B-41) with (B-42) denote the exact increment of the functional I corresponding to an arbitrary variation of the distribution control $\underset{\sim}{u}(z,t)$.

Note also that the remainder term β groups only second order terms.

B.2 State and Costate Incrementals to a Control Perturbation

The estimate of the remainder term β involves the estimates of the magnitude of $\underset{\sim}{\Delta\Phi}$ and $\underset{\sim}{\Delta\psi}$ corresponding to variations in the control vector $\underset{\sim}{u}(z,t)$.

The estimates of these quantities will be derived from the concept of characteristics developed essentially in Appendix A.

System (4-2) may be written for $\underset{\sim}{\Delta\Phi}(z,t)$ as:

$$\frac{\partial \Delta\Phi_i}{\partial t} + \sum_{j=1}^{n} a_{ij} \frac{\partial \Delta\Phi_j}{\partial z} = \Delta f_i \qquad i=1,\ldots,n \qquad \text{(B-44)}$$

Also, under the hyperbolicity condition stated for the system, a non-singular linear transformation of the unknown vector $\Delta\underset{\sim}{\phi}(z,t)$ may be proved to exist, (see Appendix A).

$$\Delta n_i = \sum_{j=1}^{n} k_{ij} \cdot \Delta\Phi_j \qquad i=1,\ldots,n \qquad \text{(B-45)}$$

which converts system (B-44) to the form,

$$\frac{\partial \Delta n_i}{\partial t} + \lambda_i \frac{\partial \Delta n_i}{\partial z} = \Delta \frac{\partial H^*}{\partial \psi_i} \qquad i=1,\ldots,n \qquad \text{(B-46)}$$

with,

$$\Delta \frac{\partial H^*}{\partial \psi_i} = \sum_{j=1}^{n} \{ k_{ij} \cdot \Delta f_j + \frac{\partial k_{ij}}{\partial t} \cdot \Delta\Phi_j + \frac{\partial(\lambda_i k_{ij})}{\partial z} \cdot \Delta\Phi_j \} - \Delta n_i \frac{\partial \lambda_i}{\partial z} \qquad \text{(B-47)}$$

Note that equation (B-46) is analogous in form to (A-14), and equation (B-47) to (A-15) of Appendix A and equation (B-46) assumes the canonical form.

In equations (B-46) and (B-47) the characteristic values $\lambda_i(z,t)$ are differentiable functions with respect to z and t and are the roots of the characteristic polynomial (A-8). The characteristic vector $k_{ij}(z,t)$ which are solutions of the homogeneous system (A-7) also possess with the characteristic roots $\lambda_i(z,t)$ the same smoothness properties as the matrix coefficients $a_{ij}(z,t)$.

Since the matrix coefficients $a_{ij}(z,t)$ are continuous and continuously differentiable with respect to z and t in the finite domain τ they are therefore also bounded there and so are the characteristic values $\lambda_i(z,t)$ and $k_{ij}(z,t)$.

Furthermore, since the vector $\underset{\sim}{f}(z,t,\underset{\sim}{\phi},\underset{\sim}{u})$ of system (4-2) possesses at least continuous first derivatives with respect to its arguments in τ,

then the vector $\underset{\sim}{f}(z,t,\underset{\sim}{\phi},\underset{\sim}{u})$ satisfies a Lipschitz condition with respect to vector $\underset{\sim}{\phi}(z,t)$ and $\underset{\sim}{u}(z,t)$ in τ [Coddington and Levinson (1955)].

Hence equation (B-47), factorable in terms of these quantities, satisfies a Lipschitz condition with respect to vectors $\underset{\sim}{\phi}(z,t)$ and $\underset{\sim}{u}(z,t)$ in τ, that is, there exist a constant $M_1 > 0$ such that,

$$\left| \frac{\partial H^*[z,t,\underset{\sim}{\eta}^1(z,t),\underset{\sim}{u}^1(z,t)]}{\partial \psi_i} - \frac{\partial H^*[z,t,\underset{\sim}{\eta}^2(z,t),\underset{\sim}{u}^2(z,t)]}{\partial \psi_i} \right| \tag{B-48}$$

$$\leq M_1 \cdot \left[\sum_{i=1}^{n} \left| \eta_i^1 - \eta_i^2 \right| + \sum_{k=1}^{r} \left| u_k^1 - u_k^2 \right| \right]$$

or since in the case considered,

$$\left| \eta_i^1 - \eta_i^2 \right| = \left| \Delta \eta_i \right| \qquad i=1,\ldots,n \tag{B-49}$$

and

$$\left| u_k^1 - u_k^2 \right| = \left| \Delta u_k \right| \qquad k=1,\ldots,n \tag{B-50}$$

equation (B-48) may be rewritten

$$\left| \frac{\Delta \partial H^*}{\partial \psi_i} \right| \leq M_1 \cdot \left[\sum_{i=1}^{n} \left| \Delta \eta_i \right| + \sum_{k=1}^{r} \left| \Delta u_k \right| \right] \tag{B-51}$$

where M_1 is a Lipschitz constant.

Since equation (B-46) may be written as,

$$\left. \frac{d\, \Delta \eta_i}{dt} \right|_{L_i} = \frac{\Delta \partial H^*}{\partial \psi_i} \qquad i=1,\ldots,n \tag{B-52}$$

with the same significance as in equation (A-24), integrating it in the sense given there, equation (B-52) becomes,

$$\Delta \eta_i(z,t) - \Delta \eta_i(z_i,t_o) = \int_{t_o}^{t} \Delta \frac{\partial H^*}{\partial \psi_i} \, d\ell \qquad i=1,\ldots,n \tag{B-53}$$

Substituting expression (B-51) in equation (B-53) and noting that $\Delta \eta_i(z_i,t_o) = 0$ gives,

$$\left|\Delta \eta_i\right| \leq M_1 \cdot \int_{t_o}^{t} \left[\sum_{i=1}^{n} \left|\Delta \eta_i\right| + \sum_{k=1}^{r} \left|\Delta u_k\right|\right] d\ell \qquad i=1,\ldots,n \tag{B-54}$$

or summing it for i=1,...,n:

$$\sum_{i=1}^{n} \left|\Delta \eta_i\right| \leq n \cdot M_1 \int_{t_o}^{t} \left[\sum_{i=1}^{n} \left|\Delta \eta_i\right| + \sum_{k=1}^{r} \left|\Delta u_k\right|\right] d\ell \tag{B-55}$$

Since this could be written in the form,

$$y(t) \leq a + \int_{t_o}^{t} b(s).y(s).ds \tag{B-56}$$

with,

$$y(s) = \sum_{i=1}^{n} \left|\Delta \eta_i\right| \geq 0 \tag{B-57}$$

$$a = n M_1 \int_{t_o}^{t} \sum_{k=1}^{r} \left|\Delta u_k\right| \, d\ell \geq 0 \tag{B-58}$$

$$b = n\, M_1 > 0 \tag{B-59}$$

a lemma on integral inequality [Lakshmikantham and Leela (1969)] instructs us that expression (B-56) may be written as,

$$y(t) \leq a \cdot \exp\left\{\int_{t_o}^{t} b(s)\, ds\right\} \tag{B-60}$$

or in terms of expression (B-55),

$$\sum_{i=1}^{n} \left|\Delta\, \eta_i\right| \leq M_2 \cdot \int_{t_o}^{t} \sum_{k=1}^{r} \left|\Delta\, u_k\right|\, d\ell \tag{B-61}$$

Finally, since,

$$\Delta\, \eta_i \leq \sum_{i=1}^{n} \left|\Delta\, \eta_i\right| \qquad i=1,\ldots,n \tag{B-62}$$

inequality (B-61) becomes,

$$\left|\Delta\, \eta_i\right| \leq M_3 \int_{t_o}^{t_f} \sum_{k=1}^{r} \left|\Delta\, u_k\right|\, d\ell \qquad i=1,\ldots,n \tag{B-63}$$

where t_f is the largest finite value of time t corresponding to the largest value of s_i in the region of integration along L_i, and M_3 is a positive constant whose value may change with i=1,...,n.

Since $\underset{\sim}{u}(z,t) \in U$, where U is a closed set, $|\Delta\, u_k|$ is a bounded quantity in τ and quantities (B-63) are also bounded there.

The characteristic vector $k_{ij}(z,t)$ being unaffected by a perturbation in control, transformation (B-45) may be used in inequalities (B-63) to yield,

$$\left|\Delta \Phi_i\right| \leq M_4 \cdot \int_{t_o}^{t_f} \sum_{k=1}^{r} \left|\Delta u_k\right| \, d\ell \qquad i=1,\ldots,n \qquad \text{(B-64)}$$

with M_4 possessing the same characteristics as M_3

Letting $\underset{\sim}{\Delta}\bar{u}$ be the largest of $|\Delta u_k|$, k=1,...,r, inequalities (B-64) reduce to,

$$|\Delta \Phi_i| \leq c_1 \cdot \Delta\bar{u} \cdot \Delta t \qquad i=1,\ldots,n \qquad \text{(B-65)}$$

where Δt represents a time interval for which some of the $|\Delta u_k|$ are non-zero, and c_1 is a positive constant whose value may change with i=1,...,n.

System (4-12) may also be written for $\underset{\sim}{\Delta}\psi(z,t)$ as,

$$\frac{\partial \Delta\psi_i}{\partial t} + \sum_{j=1}^{n} \frac{\partial\{a_{ji} \cdot \Delta\psi_j\}}{\partial z} = - \sum_{j=1}^{n} \Delta\{\psi_j \frac{\partial f_j}{\partial \Phi_i}\} \qquad i=1,\ldots,n \qquad \text{(B-66)}$$

where under the hyperbolicity condition stated for system (4-2), a non-singular linear transformation of the unknown vector $\underset{\sim}{\Delta}\psi(z,t)$ may be proved to exist, (see Appendix A),

$$\Delta \omega_s = \sum_{j=1}^{n} k'_{sj} \cdot \Delta\psi_j \qquad s=1,\ldots,n \qquad \text{(B-67)}$$

where k'_{sj} is defined by,

$$\sum_{i=1}^{n} k'_{si} \cdot a_{ji} = \lambda_s \cdot k'_{sj} \qquad s=1,\ldots,n \qquad \text{(B-68)}$$

and which converts system (B-66) to the form,

$$\frac{\Delta\,\omega_s}{\partial t} + \lambda_s \cdot \frac{\partial \Delta\,\omega_s}{\partial z} = \Delta\,\frac{\partial H^{**}}{\partial \Phi_s} \qquad s=1,\ldots,n \tag{B-69}$$

with

$$\Delta\frac{\partial H^{**}}{\partial \Phi_s} = -\sum_{i=1}^{n}\sum_{j=1}^{n} k'_{si}\,\Delta\left\{\psi_j\,\frac{\partial f_j}{\partial \Phi_i}\right\} + \sum_{i=1}^{n}\Delta\,\psi_i \cdot \frac{\partial k'_{si}}{\partial t}$$
$$+ \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ji} \cdot \Delta\,\psi_j \cdot \frac{\partial\, k'_{si}}{\partial z} - \Delta\,\omega_s \cdot \frac{\partial \lambda_s}{\partial z} \tag{B-70}$$

Note again that equation (B-68) is analogous in form to (A-14) with $\underset{\sim}{\varepsilon} \rightarrow \underset{\sim}{\Delta\omega}$ and assumes the canonical form.

All previous continuity, differentiability and boundedness arguments relative to the characteristic quantities $\lambda_s(z,t)$ and $k'_{sj}(z,t)$ and the matrix coefficients $a_{ij}(z,t)$ hold, and since the vector $f(z,t,\underset{\sim}{\Phi},\underset{\sim}{u})$ of system (4-2) is continuously twice differentiable with respect to vector $\underset{\sim}{\Phi}(z,t)$ and $\underset{\sim}{u}(z,t)$, hence $\frac{\partial f_j}{\partial \Phi_i}$ satisfies a Lipschitz condition with respect to these arguments, equations (B-70) factorable in terms of these quantities also satisfy a Lipschitz condition with respect to $\underset{\sim}{\Phi}(z,t)$ and $\underset{\sim}{u}(z,t)$.

That is, explicitly,

$$\left|\Delta\,\frac{\partial H^{**}}{\partial \Phi_i}\right| \leq M_5 \cdot \left[\sum_{i=1}^{n}\left|\Delta\,\Phi_i\right| + \sum_{k=1}^{r}\left|\Delta\,u_k\right|\right] \qquad i=1,\ldots,n \tag{B-71}$$

where M_5 is a Lipschitz constant.

Since equation (B-69) may be written as,

$$\left.\frac{d\,\Delta\,\omega_i}{dt}\right|_{L_i} = \Delta\,\frac{\partial H^{**}}{\partial \Phi_i} \qquad i=1,\ldots,n \tag{B-72}$$

with equation (B-72) having the same significance as in (A-24). Integrating equation (B-72) in the same sense given there, but backward along the characteristic L_i starting from terminal time t_f,

$$\Delta\,\omega_i(z,t) - \Delta\,\omega_i(z_i,t_f) = \int_t^{t_f} \Delta\,\frac{\partial H^{**}}{\partial \Phi_i}\,d\ell \qquad i=1,\ldots,n \qquad \text{(B-73)}$$

Substituting expression (B-71) in equation (B-73) and noting that $\Delta\,\omega_i(z_i,t_f) = 0$ gives,

$$\left|\Delta\,\omega_i\right| \leq M_5 \cdot \int_t^{t_f} \left[\sum_{i=1}^{n} \left|\Delta\,\Phi_i\right| + \sum_{k=1}^{r} \left|\Delta\,u_k\right|\right] d\ell \qquad i=1,\ldots,n \qquad \text{(B-74)}$$

Noting that results (B-64) permits to write,

$$\int_{t_o}^{t_f} \sum_{i=1}^{n} \left|\Delta\,\Phi_i\right|\,d\ell \leq n \cdot M_4.(t_f-t_o) \int_{t_o}^{t_f} \sum_{k=1}^{r} \left|\Delta\,u_k\right|\,d\ell \qquad \text{(B-75)}$$

substitution of inequality (B-75) into result (B-74) gives,

$$\Delta\,\omega_i \leq M_6 \cdot \int_{t_o}^{t_f} \sum_{k=1}^{r} \left|\Delta\,u_k\right|\,d\ell \qquad i=1,\ldots,n \qquad \text{(B-76)}$$

with

$$M_6 = \{n\,M_4(t_f-t_o) + M_5\} > 0 \qquad \text{(B-77)}$$

Since the boundedness and invariability arguments involved in the passing from inequalities (B-63) to (B-64) apply here with respect to transformations (B-69), the following results are obtainable,

$$\left|\Delta\ \psi_i\right| \leq M_7 \int_{t_o}^{t_f} \sum_{k=1}^{r} \left|\Delta\ u_k\right|\ d\ell \qquad i=1,\ldots,n \qquad \text{(B-78)}$$

where $M_7 > 0$.

Hence,

$$\left|\Delta\ \psi_i\right| \leq c_2\ .\ \Delta\bar{u}\ .\ \Delta t \qquad i=1,\ldots,n \qquad \text{(B-79)}$$

where c_2 is a positive constant whose value may change with i=1,...,n and $\Delta\bar{u}$ and Δt have the same significance as in inequalities (B-65).

B.3 The Remainder Term in the Formula for the Functional Increment

Since the validity of the following inequality is recognized [Bartle (1964)],

$$\sum_{i=1}^{n}\sum_{j=1}^{n} \left|\tau_{ij}\right|.\left|\alpha_i\right|.\left|\beta_j\right| \geq \sum_{i=1}^{n}\sum_{j=1}^{n} \tau_{ij}\ \alpha_i\ \beta_j \qquad \text{(B-80)}$$

and recalling equations (B-18) and (B-27), the expression for the remainder term (B-42) may be written accordingly as,

$$\beta \leq \int_{t_o}^{t_f} \int_{z_o}^{z_f} \{ \sum_{j=1}^{n} \sum_{k=1}^{r} \left| \frac{\partial^2 H_1}{\partial \psi_j \partial u_k} \right| . |\Delta \psi_j| . |\Delta u_k| + \sum_{i=1}^{n} \sum_{k=1}^{r} \left| \frac{\partial^2 H_1}{\partial \Phi_i \partial u_k} \right| . |\Delta \Phi_i| . |\Delta u_k|$$

$$+ \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \frac{\partial^2 H_2}{\partial \Phi_i \partial \Phi_j} \right| . |\Delta \Phi_i| . |\Delta \Phi_j| + \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \frac{\partial^2 H_2}{\partial \Phi_i \partial \psi_j} \right| . |\Delta \Phi_i| . |\Delta \psi_j|$$

$$+ \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \frac{\partial^2 H_2}{\partial \psi_i \partial \psi_j} \right| . |\Delta \psi_i| . |\Delta \psi_j| + \sum_{i=1}^{n} \sum_{k=1}^{r} \left| \frac{\partial^2 H_3}{\partial \psi_i \partial u_k} \right| . |\Delta \psi_i| . |\Delta u_k| \qquad \text{(B-81)}$$

$$+ \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \frac{\partial^2 H_3}{\partial \psi_i \partial \Phi_j} \right| . |\Delta \psi_i| . |\Delta \Phi_j| + \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \frac{\partial^2 H_3}{\partial \psi_i \partial \psi_j} \right| . |\Delta \psi_i| . |\Delta \psi_j| \} dz\, dt$$

$$+ \frac{1}{2} \int_{t_o}^{t_f} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \frac{\partial^2 G''_{2_a}}{\partial \Phi_i(z_f,t) \partial \Phi_j(z_f,t)} \right| . |\Delta \Phi_i(z_f,t)| . |\Delta \Phi_j(z_f,t)| dt$$

$$+ \frac{1}{2} \int_{z_o}^{z_f} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| \frac{\partial^2 G''_{3_a}}{\partial \Phi_i(z,t_f) . \partial \Phi_j(z,t_f)} \right| . |\Delta \Phi_i(z,t_f)| . |\Delta \Phi_j(z,t_f)| dz$$

The function H being a twice continuously differentiable function with respect to its arguments in the whole of τ, the second partial derivatives of that function are bounded in the domain of the space defined by $z, t, \underset{\sim}{\Phi}, \underset{\sim}{\psi}$ and $\underset{\sim}{u}$, and,

$$\left| \frac{\partial^2 H}{\partial \epsilon_i \partial \epsilon_j} \right| \leq M_{\alpha ij} \qquad \text{(B-82)}$$

where $M_{\alpha ij}$ is a finite positive number.

The same arguments applying to the functions G_2'' and G_3,

$$\left|\frac{\partial^2 G}{\partial \varepsilon_i \, \partial \varepsilon_j}\right| \leq M_{\beta ij} \tag{B-83}$$

Now because of the increments $|\Delta\Phi_i|$ and $|\Delta\psi_i|$ given by relations (B-65) and (B-79),

$$\left|\frac{\partial^2 H_1}{\partial \psi_j \, \partial u_k}\right| . \left|\Delta u_k\right| . \left|\Delta \psi_j\right| \leq (M_{1jk} \cdot c_2 \cdot \Delta\bar{u} \cdot \Delta t) \cdot \left|\Delta u_k\right| \tag{B-84}$$

$$\left|\frac{\partial^2 H_1}{\partial \Phi_i \, \partial u_k}\right| . \left|\Delta \Phi_i\right| . \left|\Delta u_k\right| \leq (M_{2jk} \cdot c_1 \cdot \Delta\bar{u} \cdot \Delta t) \cdot \left|\Delta u_k\right| \tag{B-85}$$

$$\left|\frac{\partial^2 H_2}{\partial \Phi_i \, \partial \Phi_j}\right| . \left|\Delta \Phi_i\right| . \left|\Delta \Phi_j\right| \leq M_{3ij} \cdot c_1^2 \cdot (\Delta\bar{u})^2 \cdot (\Delta t)^2 \tag{B-86}$$

$$\left|\frac{\partial^2 H_2}{\partial \Phi_i \, \partial \psi_j}\right| . \left|\Delta \Phi_i\right| . \left|\Delta \psi_j\right| \leq M_{4ij} \cdot c_1 \cdot c_2 \cdot (\Delta\bar{u})^2 \cdot (\Delta t)^2 \tag{B-87}$$

$$\left|\frac{\partial^2 H_2}{\partial \psi_i \, \partial \psi_j}\right| . \left|\Delta \psi_i\right| . \left|\Delta \psi_j\right| \leq M_{5ij} \cdot c_2^2 \cdot (\Delta\bar{u})^2 \cdot (\Delta t)^2 \tag{B-88}$$

$$\left|\frac{\partial^2 H_3}{\partial \psi_i \, \partial \Phi_j}\right| . \left|\Delta \psi_i\right| . \left|\Delta \Phi_j\right| \leq M_{6ij} \cdot c_1 \cdot c_2 \cdot (\Delta\bar{u})^2 \cdot (\Delta t)^2 \tag{B-89}$$

$$\left|\frac{\partial^2 H_3}{\partial \psi_i \, \partial \psi_j}\right| . \left|\Delta \psi_i\right| . \left|\Delta \psi_j\right| \leq M_{7ij} \cdot c_2^2 \cdot (\Delta\bar{u})^2 \cdot (\Delta t)^2 \tag{B-90}$$

$$\left|\frac{\partial^2 H_3}{\partial \psi_i \, \partial u_k}\right| . \left|\Delta \psi_i\right| . \left|\Delta u_k\right| \leq (M_{8ij} \cdot c_2 \cdot \Delta\bar{u} \cdot \Delta t) \cdot \left|\Delta u_k\right| \tag{B-91}$$

$$\left|\frac{\partial^2 G_{2_a}''}{\partial \Phi_i(z_f,t) \, \partial \Phi_j(z_f,t)}\right| . \left|\Delta \Phi_i(z_f,t)\right| . \left|\Delta \Phi_j(z_f,t)\right| \leq M_{9ij} . c_1^2 . (\Delta\bar{u})^2 . (\Delta t)^2 \tag{B-92}$$

$$\left|\frac{\partial^2 G_{3_a}''}{\partial \Phi_i(z,t_f) \, \partial \Phi_j(z,t_f)}\right| . \left|\Delta \Phi_i(z,t_f)\right| . \left|\Delta \Phi_j(z,t_f)\right| \leq M_{0ij} . c_1^2 . (\Delta\bar{u})^2 . (\Delta t)^2 \tag{B-93}$$

Substituting relations (B-84 to B-93) in (B-81) and rearranging,

$$\beta \leq \bar{M}_1 . (\Delta\bar{u})^2 . (\Delta t)^2 + \bar{M}_2 . (\Delta\bar{u}) . (\Delta t) \int_{t_o}^{t_f} \int_{z_o}^{z_f} \sum_{i=1}^{k} \left|\Delta u_k\right| \, dz \, dt \tag{B-94}$$

Since $\left|\Delta u_k\right| = 0$ for $t \notin \Delta t$, and letting $\Delta\bar{u}$ represent the largest value of $\left|\Delta u_k\right|$, $k=1,\ldots,r$,

$$\int_{t_o}^{t_f} \int_{z_o}^{z_f} \sum_{i=1}^{k} \left|\Delta u_k\right| \, dz \, dt \leq k \, . \, \Delta\bar{u} \, . \Delta t \, . (z_f - z_o) \tag{B-95}$$

and finally the remainder term in the formula for the functional increment is dominated in the following way,

$$\beta \leq c_3 \, . \, (\Delta\bar{u})^2 \, . \, (\Delta t)^2 \tag{B-96}$$

where c_3 is some finite-valued constant.

B.4 A Necessary Condition

The maximum principle states that the cost functional I is minimized, for an optimal control $\underset{\sim}{u}^+$,

$$\Delta I = I\,(\underset{\sim}{u}^+ + \Delta\underset{\sim}{u}) - I\,(\underset{\sim}{u}^+) \geq 0 \tag{B-97}$$

when the function H assumes a maximum:

$$\Delta H = H[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^+ + \Delta\underset{\sim}{\bar{u}}] - H[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{u}^+] \leq 0 \tag{B-98}$$

on the set of admissible control vector $\underset{\sim}{u} \in U$.

The proof of the maximum principle is established by contradiction arguments.

Proof:

Select any point $(z^0,t^0) \in \tau$ and assume that there exists an optimal control vector $\underset{\sim}{\mu}^+(z^0,t^0)$ such that,

$$\Delta H > 0 \tag{B-99}$$

Then in view of the piecewise continuity of the control $\underset{\sim}{u}(z,t)$ with respect to z and t and the continuity of the function H with respect to its arguments, there must exist some control $\bar{\underset{\sim}{\mu}}(z^0,t^0)$ continuously defined in a neighbourhood $N(z^0,t^0) \in \Delta\tau \subset \tau$ such that the following equations,

$$F_1(z,t) = H[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\underset{\sim}{\mu}^+] \qquad \text{all } (z,t) \in \Delta\tau \tag{B-100}$$

$$F_2(z,t) = H[z,t,\underset{\sim}{\phi},\underset{\sim}{\psi},\bar{\underset{\sim}{\mu}}] \qquad \text{all } (z,t) \in \Delta\tau \tag{B-101}$$

are continuous.

By assumption (B-99)

$$\Delta H = F_2(z,t) - F_1(z,t) \geq \alpha > 0 \qquad \text{all } (z,t) \in \Delta\tau \tag{B-102}$$

where $\Delta\tau = \Delta z \times \Delta t = [z_1,z_2] \times [t_1,t_2]$.

Now consider the admissible control vector $\hat{\underset{\sim}{u}}(z,t) \in U$:

$$\hat{\underset{\sim}{u}}(z,t) = \begin{cases} \underset{\sim}{\mu}^+(z,t) & \text{for all } (z,t) \notin \Delta\tau \\ \bar{\underset{\sim}{\mu}}(z,t) & \text{for all } (z,t) \in \Delta\tau \end{cases} \tag{B-103}$$

The incremental change of the cost functional I due to the application of this control vector $\hat{\underset{\sim}{u}}(z,t)$ is given by (B-41), and,

$$\Delta I = - \int_{t_1}^{t_2} \int_{z_1}^{z_2} \Delta H \, dz \, dt + \beta \tag{B-104}$$

or substituting the assumed result (B-102):

$$\Delta I \lesssim - \{ \int_{t_1}^{t_2} \int_{z_1}^{z_2} \alpha \, dz \, dt - \beta \} \tag{B-105}$$

Since the estimate of the remainder term β is available and given by (B-96),

$$\Delta I \lesssim \int_{t_1}^{t_2} \int_{z_1}^{z_2} \{ -\alpha - \frac{c_3 \, (\Delta \bar{u})^2 (\Delta t)^2}{\Delta \tau} \} \, dz \, dt \tag{B-106}$$

and that $\Delta \tau$ is proportional to Δt, it is always possible to select $\Delta \tau$ so that its second linear dimension Δz remains bounded and non-zero as $\Delta t \to 0.$, and,

$$\lim_{\Delta t \to 0} \frac{(\Delta t)^2}{\Delta \tau} = 0 \tag{B-107}$$

Hence since $\Delta \bar{u}$ is bounded, the integrand of (B-106) is always positive and:

$$\Delta I < 0 \tag{B-108}$$

and this result contradicts (B-97).

Thus (B-98) is a necessary condition that an optimal control vector $\underset{\sim}{u}^{+}(z,t) \in U$, if it exists, must obey in order to minimize functional (4-10).

According to measure theory, the integral of an integrable function over a set of measure zero is zero. Thus, when the maximum condition holds, the integrand in (B-106) may possibly be positive only on a subset $\delta\tau$ of measure zero and consequently the contribution of the integral over the subset to ΔI is zero. This proves and complete the above result.

For the case where system (4-2) is linear and the cost functional I is linear, the maximum principle or condition (B-98) is both necessary and sufficient since the partial derivative terms are such as to make expression (B-42) for the estimate of the remainder identically equal to zero.

Therefore the incremental change of the functional I due to the application of control $\underset{\sim}{u}(z,t)$ becomes,

$$\Delta I = - \int_{t_1}^{t_2} \int_{z_1}^{z_2} \Delta H \, dz \, dt \qquad \text{(B-109)}$$

and non-positive values of ΔH will lead to non-negative values for ΔI.

APPENDIX C

QUASI STEADY-STATE AND THE MAXIMUM PRINCIPLE FORMULATION

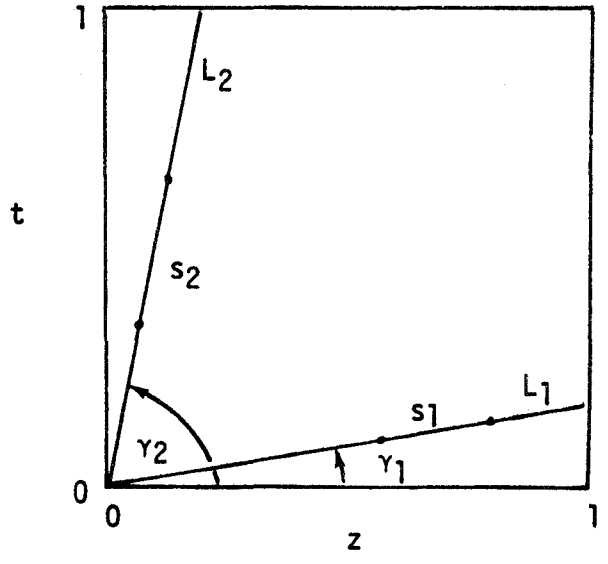
The unsteady-state system defined by equations (3-24) and (3-26) exists already in the canonical form and the characteristic roots for the system,

$$\lambda_1(z,t) = a_{11}(z,t) = (t_f/t_\Theta) \tag{C-1}$$

with

$$\lambda_2(z,t) = a_{22}(z,t) = 0. \tag{C-2}$$

are real and distinct for the whole of τ, thus making the system totally hyperbolic there (see Appendix A). Since the coefficients of the system, $a_{ij}(i,j = 1,2)$, are also constant in τ, the characteristic lines consist of two distinct families of straight lines in τ having respectively angles γ_1 and γ_2 with respect to the z axis.



where by relations (A-19),

$$\gamma_1 = \text{arc cotg } \lambda_1 \tag{C-3}$$

$$\gamma_2 = \text{arc cotg } \lambda_2 \tag{C-4}$$

The relative catalyst activity $\psi(z,t)$ may then be integrated along a linear segment s_2 of the line L_2 making an angle γ_2 with respect to axis z, or,

$$\left.\frac{d\psi}{ds_2}\right|_{L_2} = \frac{\phi}{\sqrt{1 + (\lambda_2)^2}} \tag{C-5}$$

and because by (C-2) $\lambda_2 = 0.$,

$$\left.\frac{d\psi}{ds_2}\right|_{L_2} = \left.\frac{\partial \psi(z,t)}{\partial t}\right|_z = \phi \tag{C-6}$$

and by (C-4), $\gamma_2 = \Pi/2$.

Corresponding to this angle γ_2, the result of this integration along a line L_2 parallel to the t axis gives directly the total variation of $\psi(z,t)$ in chronological time at a given station z_i of the z axis for which the initial condition $\psi(z_i,0)$ is known.

Similarly, conversion $X(z,t)$ can also be integrated along a linear segment s_1 of characteristic line L_1 which makes an angle γ_1 with respect to the z axis.

$$\left.\frac{dX}{ds_1}\right|_{L_1} = \frac{\Omega}{\sqrt{1 + (\lambda_1)^2}} \tag{C-7}$$

and for $\lambda_1 >> 1$,

$$\left.\frac{dX}{ds_1}\right|_{L_1} = \frac{\Omega}{\lambda_1} \tag{C-8}$$

Noting from (C-3) that,

$$\gamma_1 \to 0 \quad \text{for} \quad \lambda_1 \to +\infty \tag{C-9}$$

then for λ_1 sufficiently large,

$$\left.\frac{dX}{ds_1}\right|_{L_1} \approx \left.\frac{\partial X(z,t)}{\partial z}\right|_t = \frac{\Omega}{\lambda_1} \tag{C-10}$$

Since by (C-3), λ_1 represents the ratio of the total operating time t_f (hr., days) to the flow space time t_Θ of a reactor of finite length (sec., min.), this scalar is usually much larger than unity for industrial units,

$$\lambda_1 = (t_f/t_\Theta) >> 1 \tag{C-11}$$

Equation (C-10) then expresses the fact that, when condition (C-11) holds, the result of this integration along a line L_1 making an angle γ_1 with respect to axis z corresponds, at the limit for (C-9), to the result of an integration along a line parallel to axis z which would give the total variation of conversion along the flow axis z by chemical reaction along when the integration is initiated at a natural boundary such as X(0,t).

This is tantamount to say that when the space time t_Θ is small compared to the average time of total decay of the catalyst, the change in relative catalyst activity over a space time t_Θ is very nearly negligible so that in the process of integrating (C-10) along the axis z or equivalently over a space time, the relative catalyst activity at any point along this axis is not considered varying in that space time.

The chronological time scale unit for varying the relative catalyst activity $\psi(z,t)$ then becomes the space time t_Θ and represents the basic assumption of the quasi steady-state system considered here.

Hence the dynamics of a catalytic reactor process described by equations (3-24) and (3-26) and offering the characteristic (C-11) may be then well approximated by the following equations describing the state of a quasi steady-state process,

$$(t_f/t_\Theta).\ \frac{\partial X(z,t)}{\partial z} = \Omega \qquad \text{(C-12)}$$

and

$$\frac{\partial \psi(z,t)}{\partial t} = \phi \qquad \text{(C-13)}$$

with the associated initial and boundary conditions (3-27) and (3-29).

The costate equations (5-2) and (5-3) corresponding to the unsteady-state process possess the same distinct families of characteristic lines L_1 and L_2 with identical angular coefficients $1/\lambda_1$ and $1/\lambda_2$.

From this observation and following the previous discussion for condition (C-11) holding, the corresponding set of costate equations to the

quasi steady-state equations (C-12) and (C-13) is,

$$(t_f/t_\Theta).\ \frac{\partial \lambda(z,t)}{\partial z} = -\frac{\partial H}{\partial X} \tag{C-14}$$

and

$$\frac{\partial \mu(z,t)}{\partial t} = -\frac{\partial H}{\partial \psi} \tag{C-15}$$

with the associated terminal and boundary conditions (5-8) and (5-7) and the function H given by (5-1).

APPENDIX D

CHARACTERISTICS OF STATE AND COSTATE VARIABLES FOR THE QUASI STEADY STATE SYSTEM

D.1 State Variable X(z,t)

From (3-25),

$$\frac{\partial X(z,t)}{\partial z} = (t_\Theta/t_f).\{\psi(z,t).K[k(z,t)].F[X(z,t)]\} \tag{D-1}$$

integrating at constant t, from a reference station z_o to an arbitrary position z,

$$\int_{X(z_o,t)}^{X(z,t)} \frac{d\,Y}{F[Y]} = (t_\Theta/t_f).\int_{z_o}^{z} K(\varepsilon,t).\psi(\varepsilon,t)d\varepsilon \tag{D-2}$$

For continuous $X(z_o,t)$ in time, relation (D-2) indicates that a finite increase (decrease) in the value of the integral

$$\int_{z_o}^{z} K(\varepsilon,t).\psi(\varepsilon,t)d\varepsilon \tag{D-3}$$

in time would be reflected by a finite increase (decrease) of X(z,t). Similarly when integral (D-3) is continuous in time, a finite positive (negative) variation of $X(z_o,t)$ in time would be translated by a finite positive (negative) variation in X(z,t). This condition is expressed in the following way,

$$X(z,t) = P[X(z_o,t), \int_{z_o}^{z} K(\varepsilon,t).\psi(\varepsilon,t).d\varepsilon] \tag{D-4}$$

where the functional P expresses the fact that a variation in $X(z,t)$ has the same sign as a variation of $X(z_o,t)$ has or a variation of (D-3) there. For $F[X] = [1 - X]^n / C_A^{(1 - n)}$, where C_A is a constant, expression (D-4) may be explicitly formulated for $n = 1$,

$$X(z,t) = 1. - [1 - X(z_o,t)].\exp\{ - \phi_1(z,t)\} \qquad \text{(D-5)}$$

and for $n \neq 1$,

$$X(z,t) = 1. - \left\{ [1 - X(z_o,t)]^{(1 - n)} - \frac{(1 - n).\phi_1(z,t)}{C_A^{(1-n)}} \right\}^{\frac{1}{(1-n)}} \qquad \text{(D-6)}$$

with,

$$\phi_1(z,t) = (t_\Theta / t_f). \int_{z_o}^{z} K(\varepsilon,t).\psi(\varepsilon,t).d\varepsilon \qquad \text{(D-7)}$$

The state variable $X(z,t)$ is at any time t, a continuous function of z for all $z \in [0,1]$ with a continuous partial derivative $\frac{\partial X(z,t)}{\partial z}$ everywhere in Z^o except possibly at a finite set of points where the product $\{K(z,t).\psi(z,t)\}$ may have discontinuities of the first kind along the z axis.

Discontinuities in the state variable $X(z,t)$ with respect to time may occur only,

i - if $X(z_o,t)$ is discontinuous in time,

ii - a finite jump in control in time occur simultaneously along a finite length of the reactor $\Delta z \subseteq Z$,

iii - combined non-annihilating effect of (i) and (ii).

D.2 State Variabe $\psi(z,t)$

From (3-26),

$$\frac{\partial \psi(z,t)}{\partial t} = - \; k(z,t).g[\psi(z,t)] \tag{D-8}$$

integrating at constant z, from a reference time t_o to an arbitrary time t,

$$\int_{\psi(z,t_o)}^{\psi(z,t)} \frac{dy}{g[y]} = - \int_{t_o}^{t} k(z,\delta).d\delta \tag{D-9}$$

For continuous $\psi(z,t_o)$ in z, relation (D-9) indicates that a finite increase (decrease) in the value of the integral

$$\int_{t_o}^{t} k(z,\delta).d\delta \tag{D-10}$$

in z would be reflected by a finite decrease (increase) in $\psi(z,t)$. Similarly when integral (D-10) in continuous in z, a finite positive (negative) variation of $\psi(z,t_o)$ along z would be translated by a finite positive (negative) variation in $\psi(z,t)$.

For $g[\psi] = \psi^m$, expression (D-9) becomes for m = 1,

$$\psi(z,t) = \psi(z,t_o).\exp\{ - \int_{t_o}^{t} k(z,\delta).d\delta\} \qquad (D\text{-}11)$$

and for $m \neq 1$,

$$\psi(z,t) = \left\{\psi(z,t_o)^{(1 - m)} - (1 - m).\int_{t_o}^{t} k(z,\delta).d\delta\right\}^{\frac{1}{(1 - m)}} \qquad (D\text{-}12)$$

When the value of a control $k(z,t)$ at any given time in uniform everywhere in Z^o then the integral (D-10) becomes a virtual function of time only and for $m = 1$, equation (D-11) may be expressed as,

$$\psi(z,t) = \Psi_1(z).\Psi_2(t) \qquad (D\text{-}13)$$

with $\Psi_1(z) = \psi(z,t_o)$ and $\Psi_2(t) = \exp\{ - \int_{t_o}^{t} k(\delta)d\delta\}$.

The state variable $\psi(z,t)$ is at any position $z \in [0,1]$ a continuous function of time for all $t \in [0,1]$ with a continuous partial derivative $\frac{\partial \psi(z,t)}{\partial t}$ everywhere on T^o except possibly on a finite set of points where the $k(z,t)$ may have discontinuities of the first kind along the t axis.

Discontinuities in the state variable $\psi(z,t)$ with respect to distance z along the reactor may occur only,

i - if $\psi(z,t_o)$ is discontinuous along the z axis,

ii - if a finite jump in control along z exists at a location $z_s \in (0,1)$ for a finite interval of time $\Delta t \subseteq T^o$,

(iii) - combined non-annihilating effect of (i) and (ii).

D.3 Costate Variable $\lambda(z,t)$

From (5-10),

$$\frac{\partial \lambda(z,t)}{\partial z} = - (t_\Theta/t_f).\{\lambda(z,t).F'[X(z,t)].K[k(z,t)].\psi(z,t)\} \qquad (D\text{-}14)$$

and since the product,

$$\frac{\partial\ \lambda(z,t).F[X(z,t)]}{\partial z} = \lambda(z,t).\frac{\partial F[X(z,t)]}{\partial z} + F[X(z,t)].\frac{\partial \lambda(z,t)}{\partial z} \qquad (D\text{-}15)$$

and that,

$$\frac{\partial F[X(z,t)]}{\partial z} = \frac{dF[X(z,t)]}{dX(z,t)}.\frac{\partial X(z,t)}{\partial z} = F'[X(z,t)].\frac{\partial X(z,t)}{\partial z} \qquad (D\text{-}16)$$

then substituting (D-1), (D-14) and (D-16) in equation (D-15) gives,

$$\frac{\partial \lambda(z,t).F[X(z,t)]}{\partial z} = 0 \qquad (D\text{-}17)$$

and indicates that the product $\lambda(z,t).F[X(z,t)]$ is a constant everywhere in Z°. Since by (5-7), $\lambda(1,t) = (t_\Theta/t_f)$ at $z = 1$,

$$\lambda(z,t).F[X(z,t)] = (t_\Theta/t_f).F[X(1,t)] = F_1(t) \qquad (D\text{-}18)$$

D.4 Costate Variable $\mu(z,t)$

From (5-11) and (D-18)

$$\frac{\partial \mu(z,t)}{\partial t} = - \{ F_1(t).K[k(z,t)] - \mu(z,t),k(z,t).g'[\psi(z,t)]\} \qquad \text{(D-19)}$$

and since the product,

$$\frac{\partial \mu(z,t).g[\psi(z,t)]}{\partial t} = g[\psi(z,t)]\frac{\partial \mu(z,t)}{\partial t} + \mu(z,t)\frac{\partial g[\psi(z,t)]}{\partial t} \qquad \text{(D-20)}$$

and that,

$$\frac{\partial g[\psi(z,t)]}{\partial t} = \frac{dg[\psi(z,t)]}{d\psi(z,t)}.\frac{\partial \psi(z,t)}{\partial t} = g'[\psi(z,t)].\frac{\partial \psi(z,t)}{\partial t} \qquad \text{(D-21)}$$

then substituting (D-8), (D-19) and (D-21) in equation (D-20) gives,

$$\frac{\partial \mu(z,t).g[\psi(z,t)]}{\partial t} = - F_1(t).K[k(z,t)].g[\psi(z,t)] \qquad \text{(D-22)}$$

Integrating (D-22) at constant z, from a reference time t_o to an arbitrary time t,

$$\int_{\mu(z,t_o).g[\psi(z,t_o)]}^{\mu(z,t).g[\psi(z,t)]} dy = - \int_{t_o}^{t} F_1(\delta).K[k(z,\delta)].g[\psi(z,\delta)].d\delta \qquad \text{(D-23)}$$

and,

$$\mu(z,t).g[\psi(z,t)] = \mu(z,t_o).g[\psi(z,t_o)] + \int_t^{t_o} F_1(\delta).K[k(z,\delta)].$$
$$g[\psi(z,\delta)].d\delta \qquad \text{(D-24)}$$

If $t_o = 1$, then from (5-8) $\mu(z,1) = 0.$ and (D-24) reduces to,

$$\mu(z,t).g[\psi(z,t)] = \int_t^1 F_1(\delta).K[k(z,_\delta)].g[\psi(z,\delta)].d\delta \qquad \text{(D-25)}$$

D.5 Function H

From (5-1) and (D-18),

$$H = F_1(t).K[k(z,t)].\psi(z,t) - \mu(z,t).k(z,t).g[\psi(z,t)] \qquad \text{(D-26)}$$

and substituting relation (D-25),

$$H = F_1(t).K[k(z,t)].\psi(z,t) - k(z,t). \int_t^1 F_1(\delta).K[k(z,\delta)].$$
$$g[\psi(z,\delta)].d\delta \qquad \text{(D-27)}$$

APPENDIX E

Consider stations z_s where a jump in control from a policy C^* at time $t_{\bar{s}}$ to a policy C_* at time $t_{\bar{s}}$,

$$t_{\bar{s}} = \text{limit}\left\{t_s - \delta t_s\right\} \qquad \delta t_s > 0 \qquad \delta t_s \to 0 \tag{E-1}$$

then for $t < t_s$, with ΔK and Δk given by (5-112) and (5-113),

$$\Delta H(z_s,t) = - \left\{\psi(z_s,t).\Delta K.F_1(t) - \Delta k\left[.\int_{t_s}^{1} K^* F_1 g d\delta + \int_{t}^{t_s} K_* F_1 g d\delta\right]\right\} \tag{E-2}$$

or explicitly,

$$\begin{aligned}\Delta H(z_s,t) = &- \psi(z_s,t).F_1(t).K^* + k^*K_* \int_t^{t_s} F_1 g d\delta \\ &+ \psi(z_s,t).F_1(t).K_* - k_*K_* \int_t^{t_s} F_1 g d\delta \\ &+ \Delta k. \int_{t_s}^{1} K^* F_1 g d\delta\end{aligned} \tag{E-3}$$

Adding and substracting the quantity $k_*K^* \int_t^{t_s} F_1 g d\delta$, equation (E-3) becomes,

$$\Delta H(z_s,t) = - \psi(z_s,t).F_1(t).K^* + k_*K^* \int_t^{t_s} F_1 g d\delta \quad +$$

$$+ \psi(z_s,t).F_1(t).K_* - k_*K_* \int_t^{t_s} F_1 g d\delta$$
$$- k_*K^* \int_t^{t_s} F_1 g d\delta \quad + k^*K_* \int_t^{t_s} F_1 g d\delta \qquad \text{(E-4)}$$
$$+ \Delta k. \int_{t_s}^{1} K^* F_1 g d\delta$$

or recalling $\Delta(Kk)$ defined in (5-119) and factorizing,

$$\Delta H(z_s,t) = - K^* \left\{ \psi(z_s,t).F_1(t) + \int_t^{t_s} [-k_* g].F_1 d\delta \right\}$$
$$+ K_* \left\{ \psi(z_s,t).F_1(t) + \int_t^{t_s} [-k_* g].F_1 d\delta \right\} \qquad \text{(E-5)}$$
$$- \Delta(Kk). \int_t^{t_s} F_1 g d\delta \quad + \Delta k. \int_{t_s}^{1} K^* F_1 g d\delta$$

Now because using (3-26),

$$\psi(z_s,t).F_1(t) + \int_t^{t_s} [-k_* g].F_1 d\delta$$
$$= \psi(z_s,t).F_1(t) \quad + \int_t^{t_s} \left\{ \frac{\partial \psi}{\partial \delta} \right\} .F_1 d\delta$$
$$= \psi(z_s,t).F_1(t) \quad + \int_t^{t_s} \left\{ \frac{\partial \psi F_1}{\partial \delta} \right\} .d\delta - \int_t^{t_s} \left\{ \frac{dF_1}{d\delta} \right\} .\psi d\delta \qquad \text{(E-6)}$$
$$= \psi(z_s,t_s).F_1(t_s) - \int_t^{t_s} \left\{ \frac{dF_1}{d\delta} \right\} .\psi d\delta$$

equation (E-5) may be written,

$$\Delta H(z_s,t) = - K^*.\psi(z_s,t_s).F_1(t_s) + K^* \int_t^{t_s} \psi F_1' \frac{dX_1}{d\delta}. \, d\delta$$
$$+ K_*.\psi(z_s,t_s).F_1(t_s) - K_* \int_t^{t_s} \psi F_1' \frac{dX_1}{d\delta} .d\delta \qquad \text{(E-7)}$$
$$- \Delta(Kk). \int_t^{t_s} F_1 g d\delta \quad + \Delta k. \int_{t_s}^{1} K^* F_1 g d\delta$$

or factorizing, with ΔK as above,

$$\Delta H(z_s,t) = - \left\{ \psi(z_s,t_s).F_1(t_s).\Delta K - \Delta k \int_{t_s}^{1} K^* F_1 g d\delta \right\}$$
$$+ \int_t^{t_s} \left[\psi.F_1'. \frac{dX_1}{d\delta}. \Delta K - F_1 g.\Delta(Kk) \right].d\delta \qquad \text{(E-8)}$$

because,

$$\Delta H(z_s,t_s) = + \left\{ \psi(z_s,t_s).F_1(t_s).\Delta K - \Delta k. \int_{t_s}^{1} K^*.F_1 g d\delta \right\} \qquad \text{(E-9)}$$

and at the limit for $t_s^- \to t_s$, (E-2) becomes,

$$\Delta H(z_s,t_s^-) = - \left\{ \psi(z_s,t_s).F_1(t_s).\Delta K - \Delta k. \int_{t_s}^{1} K^*.F_1 g d\delta \right\} \qquad \text{(E-10)}$$

then equation (E-8) becomes for $t < t_s$,

$$\Delta H(z_s,t) = + \int_t^{t_s} \left[\psi.F_1'.\frac{dX_1}{d\delta}.\Delta K - F_1.g.\Delta(Kk) \right].d\delta + \Delta H(z_s,t_s^-) \qquad \text{(E-11)}$$

Now when considering station $z \in [0,1]$ where a jump in control has not yet occured for $t < t_s$,

$$\Delta H(z,t) = + \left\{ \psi(z,t).F_1(t).\Delta K - \Delta k.\left[\int_{t_s}^{1} K^*F_1 g d\delta + \int_t^{t_s} K^*F_1 g d\delta \right] \right\} \qquad \text{(E-12)}$$

Similarly (E-12) may be reduced to the form of (E-8),

$$\begin{aligned} \Delta H(z,t) = + & \left\{ \psi(z,t_s).F_1(t_s).\Delta K - \Delta k.\int_{t_s}^{1} K^*F_1 g d\delta \right\} \\ & - \left\{ \int_t^{t_s} \left[\psi.F_1'.\frac{dX_1}{dt}.\Delta K - F_1 g.\Delta(Kk) \right].d\delta \right\} \end{aligned} \qquad \text{(E-13)}$$

But since here no jump in control has occured, at the limit for $t_s^- \to t_s$,

$$\Delta H(z,t_s) = \Delta H(z,t_s^-) \qquad \text{(E-14)}$$

with,

$$\Delta H(z,t_s) = + \left\{ \psi(z,t_s).F_1(t_s).\Delta K - \Delta k.\int_{t_s}^{1} K^*F_1 g d\delta \right\} \qquad \text{(E-15)}$$

then (E-13) may be written,

$$\Delta H(z,t) = \Delta H(z,t_s^-) - \int_t^{t_s} \left[\psi . F_1' . \frac{dX_1}{dt} . \Delta K - F_1 . g . \Delta(Kk) \right] . d\delta \qquad \text{(E-16)}$$

APPENDIX F

The quasi steady-state approximation has been shown by Ogunye and Ray (1969_a) to be adequate except for very long tubes filled with very rapidly decaying catalyst. However, two other underlying conditions not explicitly stated in the works consulted but which are of great importance in the sense that they could destroy the validation at any time if not respected are discussed here.

The relation:

$$v.\frac{\partial X}{\partial z} \quad >> \quad \frac{\partial X}{\partial t} \tag{F-1}$$

should always be respected at any time not only as a sole function of the slow decay nature of the catalyst but also as a function of the controllable or uncontrollable variables of the process.

That is, the deterministic variation in the inlet conversion of the system, $X_o(t)$, which acts as a boundary condition for the reduced system has to be such that at any time relation (F-1) is satisfied, or:

$$\frac{dX_o(t)}{dt} = \frac{\partial X(z,t)}{\partial t}\bigg|_{z=0} \quad << \quad v.\frac{\partial X(z,t)}{\partial z}\bigg|_{z=0} \tag{F-2}$$

Secondly, the controllable variation of temperature that may come from a control action should also possess the quality that through its action relation (F-1) is satisfied at all times. This is because conversion being both a function of temperature and catalyst activity, a sudden change of temperature in time over some finite length of the reactor could violate condition (F-1).