EFFECTS OF LIQUID PHASE MIXING ON CONTROL OF
A DISTILLATION COLUMN

by 500

NORMAN C. PEREIRA

B. Sc. (Chemistry), Bombay University, India 1963
B. S. (Ch. Eng.), Tulsa University, Oklahoma 1966

A MASTER'S THESIS

submitted in partial fulfillment of the

requirements for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1969

Approved by:

L. T. Fan

Major Professor

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

During the past decade and a half, process dynamics and control, specifically optimal control, has been a subject of considerable interest to engineers in all fields. Basically an optimal control problem can be stated as follows: given equations which describe a dynamic system, determine how the systems controls must be manipulated as a function of time in order to maximize or minimize a performance criterion subject to constraints on the controls and/or on the elements of the system itself.

The problem of optimal control of distillation columns has been of continued interest to chemical engineers in recent years and all sorts of sophistication from the most recent developments in automatic control theory has been employed in solving these problems. However, nearly all of these investigations have been based on ideal models with the assumption of complete mixing in the liquid phase on each tray. And this in spite of the development of several models for the representation of liquid phase mixing on distillation trays (see the book by Holland [1]). The present study was motivated by the belief that the effect of liquid phase mixing on the optimal control of distillation columns has not been sufficiently highlighted in the past. This thesis is intended to be a contribution toward obtaining a better understanding of the problems involved in obtaining an optimal control policy for a distillation column wherein the liquid phase mixing on each tray is described by the so-called mixing pool model rather than the conventional completely mixed tray.

The system studied in this work is a two tray column separating a binary mixture wherein the stillpot acts as the bottom tray while the top tray serves as a rectifier. The special feature of this column is that the top tray is not considered as an ideal tray with complete mixing, instead it is considered as being divided into stages or pools, each pool consisting of completely mixed liquid. This is Kirschbaum's [2] assumption that there are pools of liquid on the tray which are completely mixed. The so-called mixing pool model is described as being divided into a number of completely mixed stages or pools [3, 4]. The concentration gradient across the tray is assumed to be made up of a series of pools with each mixing pool having a uniform composition. For a very large number of very small pools, the concentration gradient becomes continuous and plug flow exists. Conversely for a tray that is completely mixed, there is no concentration gradient and the entire tray has a uniform composition. These two limiting cases, however, may not be realized in practice. The effect of the degree of mixing indicated by the number of mixing pools, on the control policy of the column ~~is~~ the chief purpose of this investigation.

For the sake of comparison, a second system which is referred to as the "reference system" is also considered in this work. It is identical to the system under consideration except for the top tray which is a conventional ideal tray with complete mixing, i.e. with a single pool. This system serves as a basis for comparison in this investigation.

The procedure used here is to consider a single specific example wherein the system suffers a disturbance through the feed composition which in turn displaces the overhead distillate composition from its steady state, and then to apply Pontryagin's Maximum Principle in order to obtain the control policy which will return the overhead composition to its steady state value in the shortest possible time (time optimal problem). An extension is also made to the case where the deviation from the steady state composition is kept at a minimum. We assume that control is effected by manipulation of the overhead reflux flow rate.

The basic theoretical reference on the Maximum Principle is the book by Pontryagin and his co-workers [5]. A good elementary account of the Maximum Principle in both continuous and discrete form, along with numerous engineering applications can be found in the two works by Fan et al [6, 7]. While many significant applications of the Maximum Principle have been demonstrated in other engineering fields, it is only during the past few years that chemical engineers have begun to apply this mathematical theory to problems of chemical engineering importance.

One of the first and most extensive of all studies in this area was accomplished by Siebenthal and Aris [8]. They treated the optimal regulation of a continuous stirred tank reactor. Coward [9] in his work on the time optimal problem, is among the early investigators of the Maximum Principle as applied to distillation.

In this study the Maximum Principle coupled with certain numerical techniques is employed for the purpose of determining the optimal control policy. The mathematical models used are adequate to represent the phenomenon being investigated without having to go into the complexities of either the hydrodynamics or the energy balance of the system.

Chapter 2 deals with the analysis of the reference system and here a control policy is arrived at for the regulation of the overhead reflux rate for the time optimal problem. In Chapter 3 a similar analysis is carried out with the mixing pool model with two pools or tanks in series, wherein the parameters retain the same values as those in Chapter 2 except for the introduction of the mixing pool model in place of the conventional completely mixed tray. Once more a control policy is derived for the regulation of the overhead reflux rate for the time optimal problem. In Chapter 4 an extension is made to the case where the control is optimum in the sense of minimum total deviation. First the control policy is obtained for the reference system and then for the mixing pool model system. Chapter 5 summarizes the various results from Chapters 2, 3 and 4 and these results are then analyzed and conclusions drawn. Also several supporting appendices deal with the analog computer flow charts and digital computer programs, derivation of the Maximum Principle algorithm and steady state analyses of the systems considered in Chapters 2, 3 and 4.

CHAPTER 2

THE REFERENCE SYSTEM

In this chapter the reference system is considered. Initially the performance equations of the system are derived. The exact nature of the problem stated and finally the application of the Maximum Principle and the derivation of the optimal control policy terminates the chapter.

1. DEVELOPMENT OF PERFORMANCE EQUATIONS.

The assumptions and column characteristics involved in the derivation of performance equations are listed below.

(a) A column with two theoretical trays including the stillpot and using a total condenser, is to be considered.

(b) The column is separating a binary mixture assuming a linear vapor-liquid equilibrium relationship, i.e., $y_i = mx_i + c$.

(c) The top tray and the stillpot show constant molal holdup which is invariant with time.

(d) There is constant molal overflow, i.e., liquid and vapor flows from tray to tray are constant.

(e) Vapor holdup is assumed negligible.

(f) Adequate cooling water and steam are available.

(g) To permit ample boiling surface, the stillpot holdup is assumed to be 2.5 times the holdup on the top tray.

(h) The feed is a completely condensed liquid at saturation.

The essential features of the system along with the various flow streams are shown in Figure 1. The feed is introduced

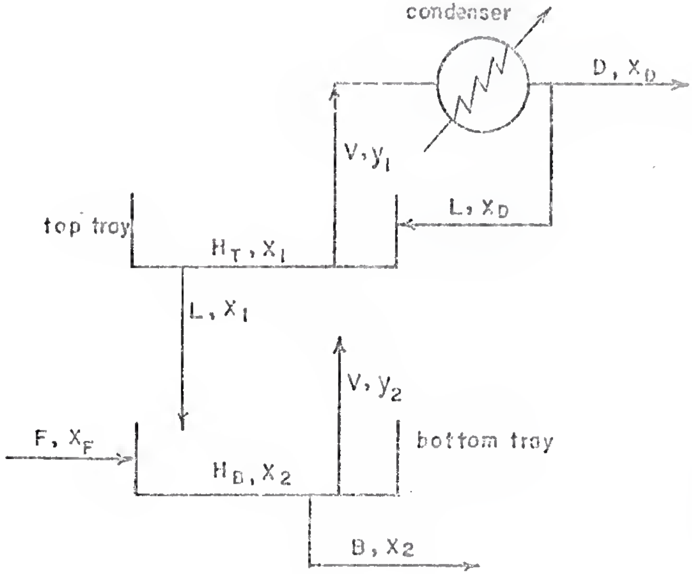


Fig. 1. Distillation column with top tray described by a single completely mixed tank (Reference-System).

directly into the stillpot as a condensed saturated liquid. In the stillpot heat is transferred to the liquid and the vapor leaving the stillpot passes upward through the rectifying section which consists of a single theoretical tray (a single completely mixed tray). The overhead vapor is completely condensed and part of the resulting liquid is drawn off as overhead product while the rest of the liquid is returned to the top tray as reflux. Liquid also leaves the reboiler and is drawn off as bottoms product.

On the basis of the above assumptions and description the mathematical relationships between the various variables can now be derived. The dynamic behavior of the column in the transient stato may be written in the differential form by performing a light component balance on each tray along with overall material and light component balances over the entire system as follows; (see Figures 2 and 3).

For the top tray, the light component balance gives

Input - Output = Accumulation

$$Lx_D + Vy_2 - Lx_1 - Vy_1 = H_T \frac{dx_1}{dt}.$$

Since

$$x_D = y_1 = mx_1 + c$$

and

$$y_2 = mx_2 + c,$$

we have

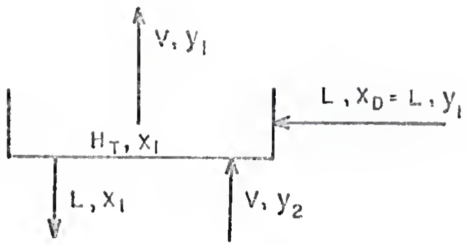


Fig. 2 Material balance streams for top tray.

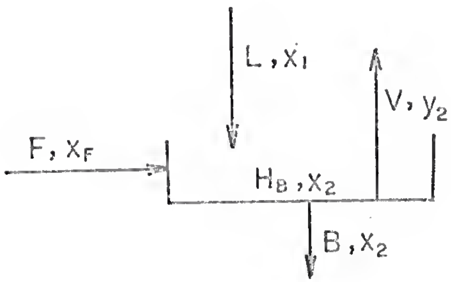


Fig. 3 Material balance streams for bottom tray.

$$L(mx_1 + c) + V(mx_2 + c) - Lx_1 - V(mx_1 + c) = H_T \frac{dx_1}{dt}$$

which on rearranging yields

$$H_T \frac{dx_1}{dt} = Lmx_1 + Lc + Vmx_2 + Vc - Lx_1 - Vmx_1 - Vc$$

and finally

$$\frac{dx_1}{dt} = \frac{(Lm - L - Vm)}{H_T} x_1 + \frac{Vm}{H_T} x_2 + \frac{Lc}{H_T} \tag{1}$$

For the bottom tray, the light component balance gives

Input - Output = Accumulation

$$Lx_1 + Fx_F - Vy_2 - Bx_2 = H_B \frac{dx_2}{dt}$$

Hence

$$H_B \frac{dx_2}{dt} = Lx_1 + Fx_F - V(mx_2 + c) - Bx_2$$

A total balance around the bottom tray shows that

$$B = F + L - V \tag{1a}$$

whereby

$$H_B \frac{dx_2}{dt} = Lx_1 + Fx_F - Vmx_2 - Vc - Fx_2 - Lx_2 + Vx_2$$

which on rearranging yields

$$\frac{dx_2}{dt} = \frac{Lx_1}{H_B} - \frac{(Vm + F + L - V)}{H_B} x_2 + \frac{Fx_F}{H_B} - \frac{Vc}{H_B} \tag{2}$$

The overall flow rate balance around the entire system gives

$$F = D + B \tag{3}$$

while the overall light component balance around the entire system, gives

$$Fx_F = Dx_D + Bx_2 \tag{3a}$$

Equations (1) and (2) describe the unsteady state behavior of the system.

The following specific values are assigned to the various parameters of the system.

$$F = 0.5 \text{ lb mole/min.} \qquad x_F = 0.65$$

$$L = 1 \text{ lb mole/min.} \qquad H_T = 1 \text{ lb mole} \tag{4}$$

$$V = 1.33 \text{ lb moles/min.} \qquad H_B = 2.5 \text{ lb moles}$$

The linear vapor-liquid equilibrium employed is

$$y_i = 0.44\, x_i + 0.56, \qquad i = 1,\ 2 \tag{4a}$$

Equations (1) and (2) have been used for simulation on an EAI TR48 analog computer to obtain several transient responses and phase plane plots. The analog computer flow charts and scaled equations are given in Appendix A. Also for the purposes of determining the physically realizable bounds of the system, the steady state and limiting case analyses of the system have been carried out. The results of the analyses are given in detail in Appendix B.

2. NATURE OF THE PROBLEM.

Using the parameter values established in section 1, the set of simultaneous equations, equations (1) and (2) with the right hand side set equal to zero can be solved to obtain the steady state values of x_1 and x_2, which represent the liquid composition of the top tray and the liquid composition of the bottom tray and also the product stream, respectively. The results are

$$x_1 = 0.6300 \tag{5}$$

and

$$x_2 = 0.2767 \tag{6}$$

Since

$$x_D = y_1 = mx_1 + c,$$

we have

$$\begin{aligned} x_D &= 0.44 \times 0.6300 + 0.56 \\ &= 0.837 \end{aligned} \tag{7}$$

If, at an instant, the feed composition x_F is instantaneously changed from its steady state value of 0.65, this change will constitute a disturbance to the overall system which in turn will eventually result in a new steady state.

Let the initial steady state ($x_1 = 0.6300$, $x_2 = 0.2767$) corresponding to $x_F = 0.65$ be designated by S_1, and at some instant let x_F be instantaneously increased to $x_F = 0.75$, (i.e. we're assuming a known disturbance to have occurred). As a result of this disturbance, x_D will tend to approach a new steady state value as can be seen in Figure 4 by the path OP. It is possible to determine a value of reflux rate L which will steer x_D from a certain point on the path, say the point P, back to its initial steady state value along PQ asymptotically. However, a better policy would be to change the reflux L not at P but at O, and thus steer x_D to its desired steady state value along ONR thereby resulting in a time saving of OQ less OR. Such a value of the reflux rate can be obtained from equations (1), (2) and (3).

From equation (3) we have

$$Fx_F = Dx_D + Bx_2$$

$$= (V - L)y_1 + (F + L - V)x_2$$

$$= (V - L)(mx_1 + c) + (F + L - V)x_2$$

This leads to

$$x_2 = \frac{Fx_F - (V - L)(mx_1 + c)}{F + L - V} \tag{8}$$

From equation (1), at steady state, we get

$$L = \frac{V(mx_1 - mx_2)}{mx_1 + c - x_1} \tag{9}$$

and from equation (2) at steady state we obtain

$$L = \frac{Vc - Fx_F - Vx_2 + Vmx_2 + Fx_2}{x_1 - x_2} \tag{10}$$

where equations (8) and (10) contain the new value of x_F.

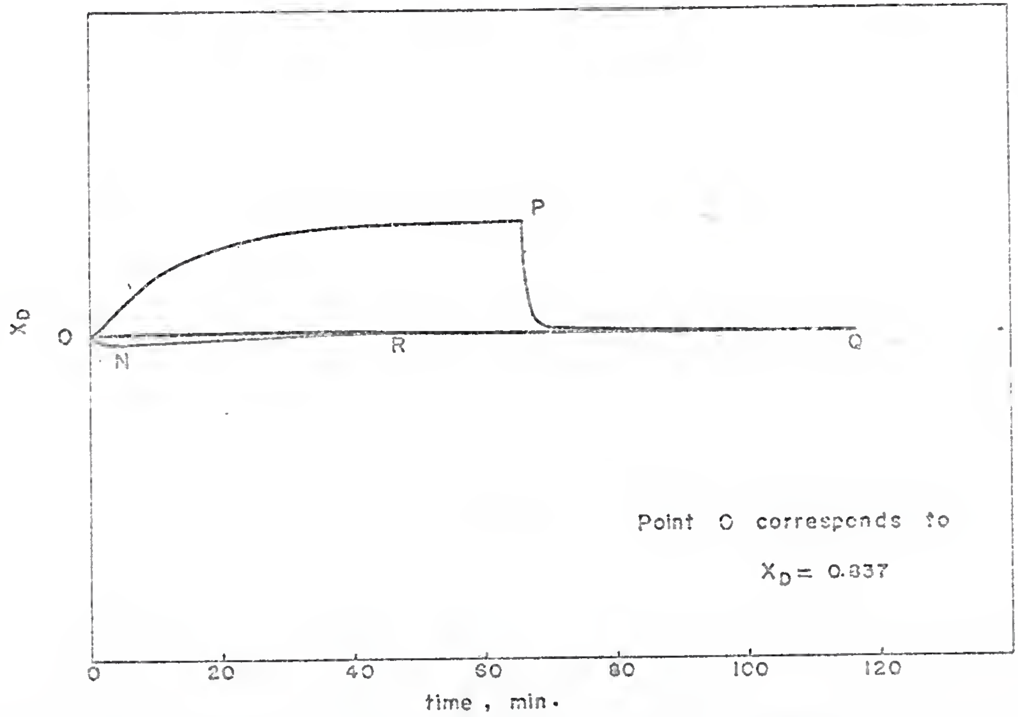


Fig. 4 Displacement and asymptotic restoration of X_D.

By a trial and error method, an L is first assumed and x_2 is calculated from equation (8). Next this value of x_2 is used in equations (9) and (10) and L is calculated from each of equations (9) and (10) and checked with the original assumed value of L. The L that satisfies equations (8), (9), and (10) shall be designated L'. The value of L' for the reference system has been found to be 0.9152 lb moles/min and the steady state resulting from it is $S_2 = (x_1 = 0.6300,\ x_2 = 0.3067)$ The increased value of x_2 is consistent with the material balance since the feed composition has been increased from 0.65 to 0.75. It can be seen from Figure 4 that the overhead composition x_D can be returned to it's initial undisturbed state in at least two different ways, one of which (path ONR) achieves the objective in a shorter time than the other. However, even the use of path ONR takes a considerable amount of time, almost to the extent that it becomes impractical to wait for x_D to return to its undisturbed state. Hence a control policy has to be devised for the manipulation of L whereby x_D is restored to its undisturbed state in the shortest possible time. This is what constitutes time optimality.

3. APPLICATION OF THE MAXIMUM PRINCIPLE ALGORITHM.

The Maximum Principle will now be applied to the reference system so as to investigate how the reflux rate should be manipulated in order to attain the state S_2 in the shortest possible time. A complete derivation of the Maximum Principle Algorithm is discussed in the Appendix C. Stating the problem more explicitly we have:

Given a system with the performance equations

$$\frac{dx_1}{dt} = \frac{(Lm - Vm - L)}{H_T} x_1 + \frac{Vm}{H_T} x_2 + \frac{Lc}{H_T} \tag{11}$$

$$\frac{dx_2}{dt} = \frac{Lx_1}{H_B} - \frac{(Vm + F + L - V)}{H_B} x_2 + \frac{Fx_F - Vc}{H_B}$$

we wish to determine $L(t)$ which moves the system from the initial state at $S_1 = (x_1 = 0.6300,\ x_2 = 0.2767)$ to the final state at $S_2 = (x_1 = 0.6300,\ x_2 = 0.3067)$ in a minimum period of time. In other words we wish to determine $L(t)$ so as to minimize the objective function S where

$$S = \int_0^T dt \tag{12}$$

where T is unspecified. Physical realizability of the system requires that the range of the control $L(t)$ must be finite (cf. Appendix B), that is,

$$L_{min} \leq L \leq L_{max} \tag{13}$$

Operation at the lower limit corresponds to the minimum reflux $L = L_{min}$, and operation at the upper limit corresponds to the maximum reflux $L = L_{max}$.

If we introduce an additional state variable such that

$$x_3(T) = \int_0^T dt$$

we have

$$\frac{dx_3}{dt} = 1; \qquad x_3(0) = 0 \tag{14}$$

The Hamiltonian function is defined as [see equation (C-8)]

$$H = \frac{(Lm - Vm - L)}{H_T} x_1 z_1 + \frac{Vmx_2}{H_T} z_1 + \frac{Lcz_1}{H_T} + \frac{L}{H_B} x_1 z_2$$

$$- \frac{(Vm + F + L - V)}{H_B} x_2 z_2 + (\frac{Fx_F - Vc}{H_B}) z_2 + z_3 \tag{15}$$

The adjoint differential system is [see equation (C-9)]

$$\frac{dz_1}{dt} = - \frac{(Lm - Vm - L)}{H_T} z_1 - \frac{L}{H_B} z_2 \tag{16}$$

$$\frac{dz_2}{dt} = - \frac{Vmz_1}{H_T} + \frac{(Vm + F + L - V)}{H_B} z_2 \tag{17}$$

$$\frac{dz_3}{dt} = 0 \tag{18}$$

The boundary conditions on the adjoint variables are [see equation (C-9)]

$$\begin{array}{llll} z_1\ (0) & \text{unspecified} & z_1\ (T) & \text{unspecified} \\ z_2\ (0) & \text{unspecified} & z_2\ (T) & \text{unspecified} \\ z_3\ (0) & \text{unspecified} & z_3\ (T) & = \quad 1 \end{array} \tag{19}$$

Equation (18) along with the final condition on $z_3(t)$ implies

$$z_3 = 1, \qquad 0 \leq t \leq T \tag{20}$$

The fact that the final time T is unfixed implies, at every moment

$$\min H = \left(\frac{mz_1x_1}{H_T} - \frac{x_1z_1}{H_T} + \frac{cz_1}{H_T} + \frac{x_1z_2}{H_B} - \frac{x_2z_2}{H_B}\right)L + \frac{Vmx_2z_1}{H_T}$$
$$- \frac{Vmx_1z_1}{H_T} - \frac{Vmx_2z_2}{H_B} - \frac{(F - V)x_2z_2}{H_B} + \frac{(Fx_F - Vc)z_2}{H_B}$$
$$+ 1 = 0 \tag{21}$$

[see equation (A-39)]. Also the Hamiltonian has been written so as to show it linear in the control variable L. Inspection of the Hamiltonian allows us to determine the basic structure of the time optimal control policy as being a bang-bang policy. That is, the control variable L assumes either its maximum value L_{max} or its minimum value L_{min} as the system is transferred from an initial state to the specified final state. Of course, once the specified final state is reached, the control variable must be switched once again to L' to maintain the new steady state. The conditions for the Hamiltonian to be a minimum are

$$L = L_{max} \quad \text{if } \left(\frac{mz_1x_1}{H_T} - \frac{x_1z_1}{H_T} + \frac{cz_1}{H_T} + \frac{x_1z_2}{H_B} - \frac{x_2z_2}{H_B}\right) < 0$$
$$L = L_{min} \quad \text{if } \left(\frac{mz_1x_1}{H_T} - \frac{x_1z_1}{H_T} + \frac{cz_1}{H_T} + \frac{x_1z_2}{H_B} - \frac{x_2z_2}{H_B}\right) > 0 \tag{21a}$$

In the case where the coefficient of L (sometimes known as the switching function) vanishes over a finite length of time we have the possibility of singular control. In the likelihood of singular control the control variable may take on values which are intermediate to L_{max} and L_{min}; hence the name intermediate control is also used in place of singular control.

The Maximum Principle now requires that the system equations, equations (11) and (14), be integrated simultaneously with the adjoint equations, equations (16) and (17) such that the two point boundary conditions

$$\begin{array}{ll} x_1(0) = 0.6300 & x_1(T) = 0.6300 \\ x_2(0) = 0.2767 & x_2(T) = 0.3067 \\ x_3(0) = 0. & x_3(T) \text{ unfixed} \\ z_1(0) \text{ unfixed} & z_1(T) \text{ unfixed} \\ z_2(0) \text{ unfixed} & z_2(T) \text{ unfixed} \end{array} \tag{21b}$$

are satisfied and assures us that the time optimal control is one which minimizes the Hamiltonian at every point of its response. Since the final time is unspecified this minimum of the Hamiltonian is zero as indicated in equation 21 [also see equation (C-39)].

4. COMPUTATIONAL PROCEDURES

The numerical solution of this problem involves guessing the initial values of z_1 and z_2 such that the final conditions $x_1(T)$ and $x_2(T)$ may be reached simultaneously when the set of five differential equations is integrated in a forward manner. Actually the guesswork can be reduced to the guessing of only one of the initial values - either $z_1(0)$ or $z_2(0)$ - by making use of equation (21). If all the parameter values specified in equations (4) and (4a) (except L) are substituted into equation (21) along with the initial values of x_1 and x_2, we get

$$[0.2773z_1(0) - 0.6300z_1(0) + 0.56z_1(0) + 0.2521z_2(0) - 0.1108z_2(0)]L(0) + 0.1625z_1(0) - 0.3696z_1(0) - 0.065z_2(0) + 0.0923z_2(0) - 0.1486z_2(0) + 1 = 0$$

which on rearranging yields

$$(0.2071L(0) - 0.2071)z_1(0) + (0.1413L(0) - 0.1213)z_2(0) + 1 = 0$$

or

$$z_1(0) = - \frac{1 + [0.1413L(0) - 0.1213]z_2(0)}{0.2071L(0) - 0.2071} \qquad (22)$$

This equation indicates that it suffices to guess the initial value of z_2 only, since $z_1(0)$ now is dependent on $z_2(0)$ and $L(0)$.

The system equations, equations (11), (16) and (17) have been integrated on an IBM system 360 computer with the help of the IBM supplied subroutine RKGS (Runge-Kutta Gill subroutine). The RKGS subroutine solves a set of simultaneous differential equations with given initial conditions. The overall logic flow diagram for the trial and error solution can be seen in Figure 5 where the following procedure is indicated in the corresponding numbered boxes.

(1) The known initial values namely, $x_1(0)$, $x_2(0)$ and $x_3(0)$ are read in.

(2) A choice of either L_{max} or L_{min} is made for L.

(3) The initial value of z_2 is assumed.

(4) The corresponding initial value of z_1 is calculated from

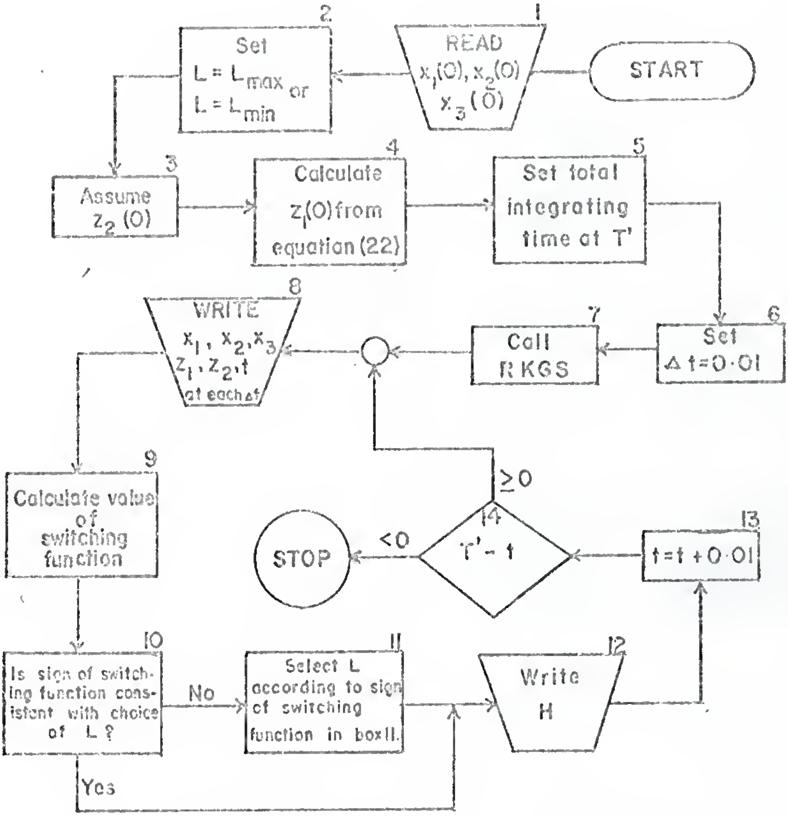


Fig. 5. Computer logic diagram for trial and error solution of equations (11), (14), (16) and (17).

equation (22).

(5) The integration procedure is set to terminate at some large value T'.

(6) The increment in time is set at 0.01.

(7) Subroutine RKGS is called, and the integration commences. Here mention must be made that the commands to be executed in boxes 8 to 14 inclusive, take place over each t.

(8) The current values of x_1, x_2, x_3, z_1, z_2 and t are written out.

(9) The value of the switching function is calculated.

(10) The sign of the switching function is checked for consistency with the choice of L in box 2. If the choice of L is consistent with current sign, then command transfers to box 12, if not, to box 11.

(11) A choice of L is made to match the current sign of the switching function.

(12) The current value of the Hamiltonian is written out. The reason for doing this is to check whether H maintains a constant value of zero during the transient response.

(13) The time is incremented to the next higher value.

(14) The current value of time is compared with the total integrating time specified in box 5.

For the initial guess $z_2(0)$ to be the right one, the desired final values of x_1 and x_2 should occur at the same Δt. Also it is imperative that the Hamiltonian vanish throughout the optimal transient response.

The above procedure of calculation was applied to the reference system after selecting suitable values for L_{max} and L_{min}. Initially a preliminary case was investigated wherein L_{max} was set at 0.980 and L_{min} at 0.896. The optimal policy was found to be to start with L_{max} and then to switch to L_{min} after 2.46 minutes. The final state was attained via L_{min} in an additional 1.28 minutes. For the preliminary case above, the values of L_{max} and L_{min} were selected in an arbitrary manner; however, for furthur analysis of the system, L_{max} and L_{min} were selected in a manner symmetric about $L' = 0.9152$, (which is the reflux rate that maintains the desired final state) as seen in Figure 6. A point symmetric with $L = 0.833$ on the right side of L' was found to be $L = 0.9974$. Hence, $L = 0.833$ and $L = 0.9974$ were taken as the 0% and 100% points of the range within which L_{max} and L_{min} were selected. (The maximum and minimum bounds on L have been established in Appendix B). The different cases investigated were:

Case 1 $L_{min} = 0.8330$ $L_{max} = 0.9974$

Case 2 $L_{min} = 0.86588$ $L_{max} = 0.96452$

Case 3 $L_{min} = 0.89876$ $L_{max} = 0.93164$

In each of the above cases the average of L_{max} and L_{min} is L'.

Case 1 L_{max} = 0.99740 100 %
L_{min} = 0.83300 0 %

Case 2 L_{max} = 0.96452 80 %
L_{min} = 0.86588 20 %

Case 3 L_{max} = 0.93164 60 %
L_{min} = 0.89876 40 %

Case 4 L_{max} = 1.3330
L_{min} = 0.8330

Fig. 6. Physical bounds within which L is constrained for cases 1, 2, 3 and 4.

In addition to the above three cases a fourth case was investigated wherein the whole horizontal line in Figure 6 was included. For this case we have

$$\text{Case 4} \quad L_{min} = 0.833 \quad L_{max} = 1.333$$

Apart from the preliminary case where $L_{max} = 0.980$ and $L_{min} = 0.896$, Case 1 was also solved by the trial and error method outlined in Figure 5, wherein the adjoint equations were solved along with the system equations. However, this method was found to be tedious and time consuming and in place of it the phase plane method, used by Siebenthal and Aris [8], was employed to obtain the solutions for Cases 2, 3, and 4. In using the phase plane method Pontryagin's Maximum Principle was employed only to find that bang-bang control was necessary and then the adjoint equations were discarded and phase plane diagrams were used to obtain the solutions. This enables us to circumvent to some extent, the inherent difficulties of the two point boundary value problem. Before going into the description of the phase plane method, the following two facts are worth noting.

1. The state equations are autonomous, (i.e. time does not appear explicitly on the right hand side of the equations) Theorems on the uniqueness of solutions for autonomous systems [10] guarantee that for a given value of the control variable L, trajectories in the phase plane do not intersect at any point except at the steady state point corresponding to L.

2. It is known that during the transient period, the optimal control policy is bang-bang and furthermore, the number of switches in the value of the control variable will be kept at a minimum since the time taken to get from the initial state to the final state would increase as the number of switches is increased [11].

In Figures 7, 8, and 9 phase planes are presented for the preliminary case where the values of $L_{min} = 0.896$, $L' = 0.9152$ and $L_{max} = 0.980$ respectively, (this is the preliminary case already solved by the trial and error method on the digital computer). In Figure 7, point A is the steady state point, and in Figure 9, point B is the steady state point. The steady state point S_2 on Figure 8 is the desired final state. This point is also shown on Figures 7 and 9. Since the system is autonomous, only one curve passes through the point S_2 in the Figures 7 and 9 [10] these curves are lettered DS_2 and ES_2 respectively. If Figures 7 and 9 are superimposed as shown in Figure 10, it becomes obvious that there are an infinite number of paths consisting of alternating L_{min} and L_{max} response segments which connect a given initial point to the point S_2. However, all of these possible paths approach S_2 via either the L_{max} segment ES_2 or the L_{min} segment DS_2.

Closer inspection of Figure 10 shows that it is possible to connect every point on the x_1, x_2 plane to the point S_2 by means of a path consisting of one L_{max} and one L_{min} segment or vice versa. Such a path is S_1FS_2 in Figure 10 where S_1 corresponds to the initial state of the reference system

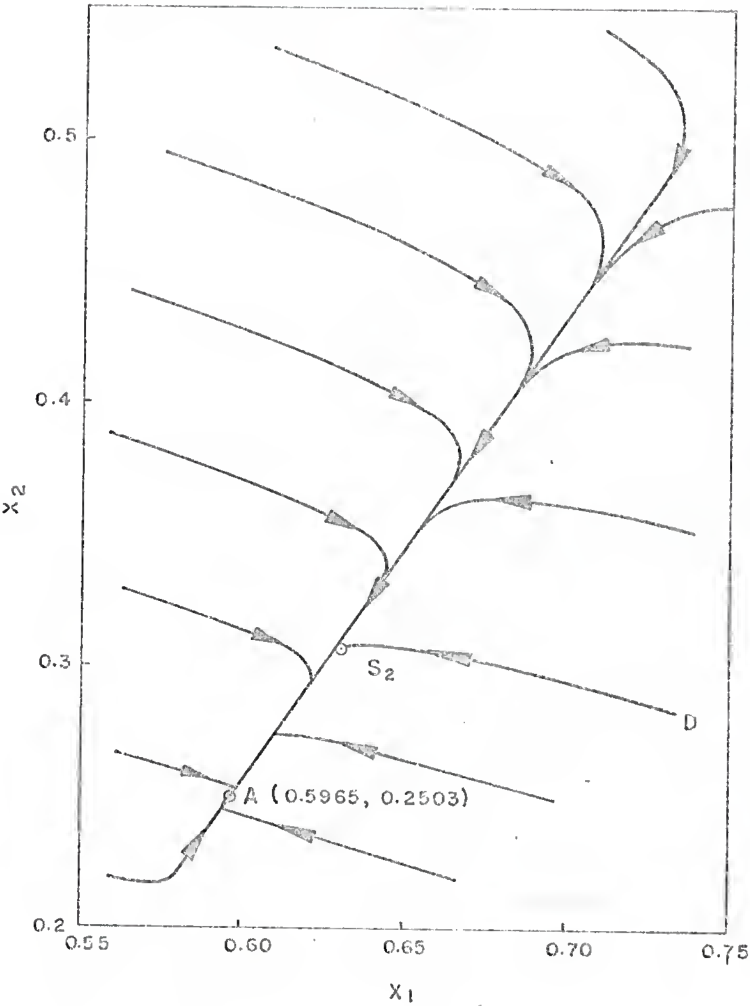


Fig. 7. Phase plane of reference system with L = 0·896 lb moles/min. (Preliminary Case).

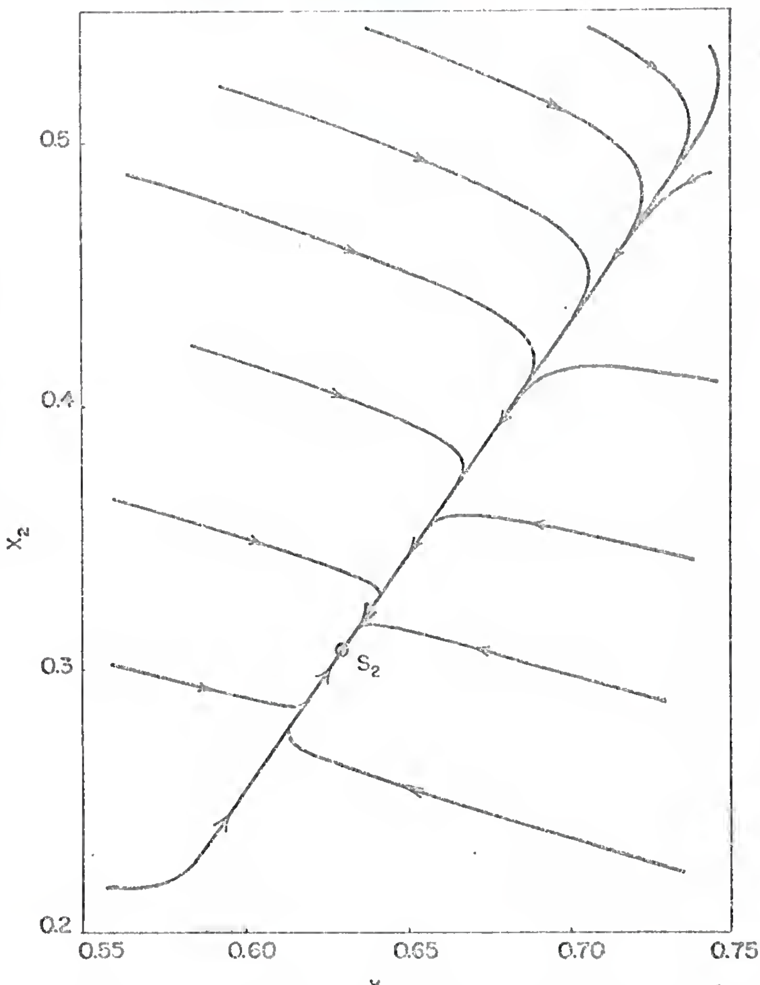


Fig. 8. Phase Plane of Reference System with $L_1' = 0.9152$ lb. moles / min. Preliminary Case.

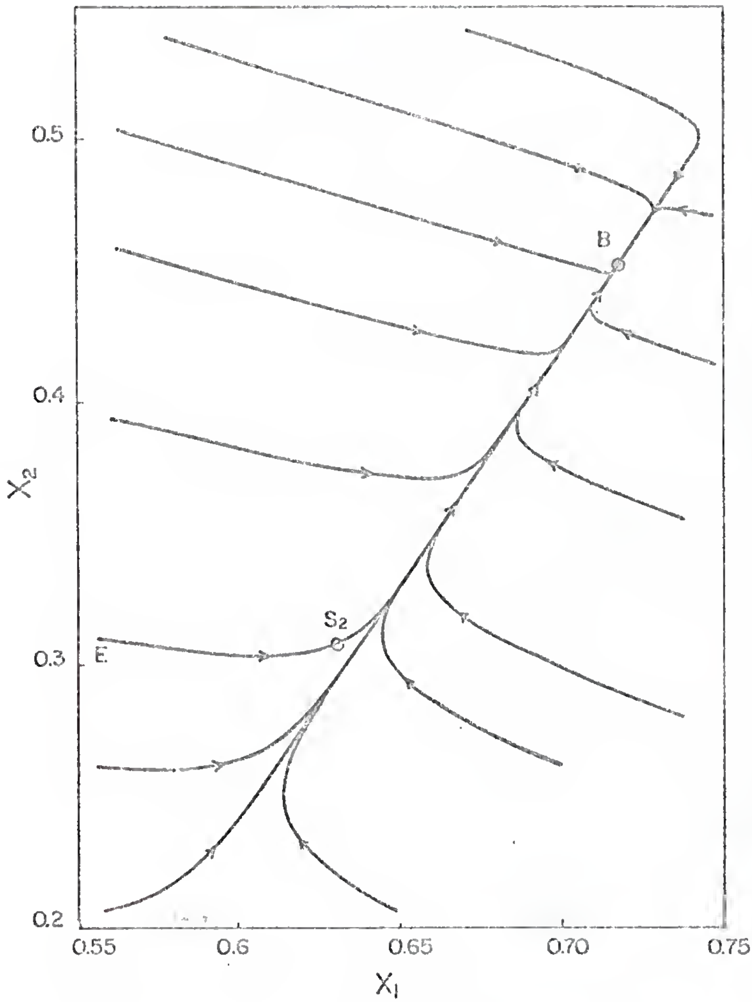


Fig. 9. Phase plane of reference system with L_{max} = 0.980 lb.moles/min. (Preliminary Case).

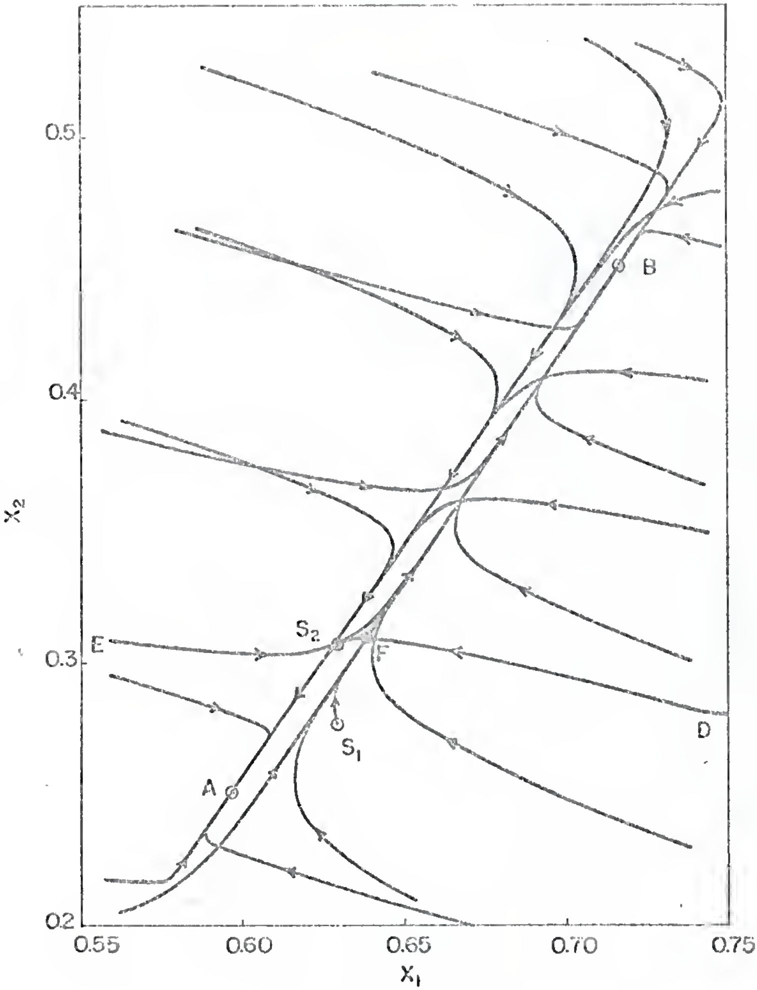


Fig. 10. Superimposition of Figures 7 and 9 (Preliminary Case).

(0.6300, 0.2767). This path has only one switch at point F. Also the path S_1FS_2 confirms the phase plane method of solution since the point F agrees with the point in the digital computer solution, previously obtained, at which the switching function changes sign and the control policy switches from L_{max} to L_{min}. Hence, the only control policies which satisfy the Maximum Principle equations contain just one control switch which occurs when the response intersects the curve DS_2E in Figure 10. Curve DS_2E is called the "switching boundary" due to the fact that it divides the phase plane into regions of L_{max} and L_{min} operation. In Figure 10, operation in the region above DS_2E is with L_{min} while operation in the region below DS_2E is with L_{max}. This method of phase plane analysis was also used in obtaining the optimal control policy for Cases 1, 2, 3, and 4 as follows;

First the phase plane plots were obtained on an analog computer by integrating the system equations only and then phase plane plots similar to Figure 10 were obtained individually for the 4 cases by superimposition of L_{min} and L_{max} response phase planes. These can be seen in Figures 11, 12, 13 and 14. Next, on the digital computer, the system equations were first integrated forward in time from the point S, using L_{max} as the control variable, and next integrated backward in time from the point S_2, using L_{min} as the control variable. By comparing the computer outputs the common point F was located. Once more a forward integration was carried out from S_1 and using L_{max} as control variable. Also this time, a command was included for the control variable to switch from L_{max} to L_{min} when F was

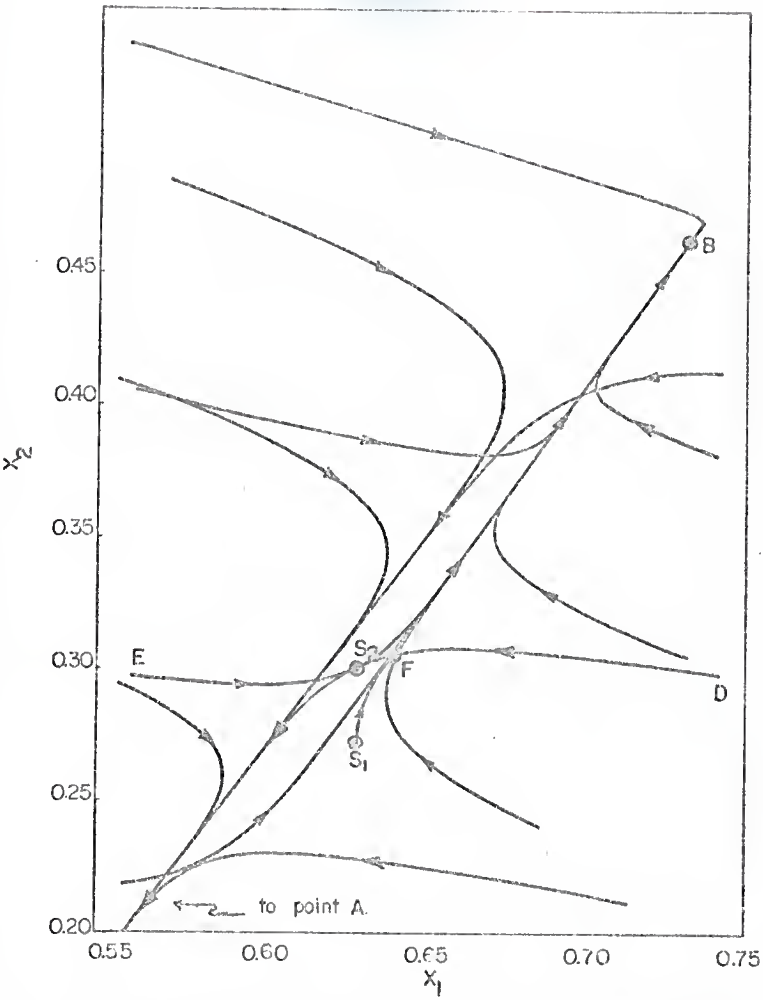


Fig. 11. Superimposition of L_{max} and L_{min} response phase planes for Case I. Paths directed to point B are L_{max} response curves and paths directed to point A are L_{min} response curves.

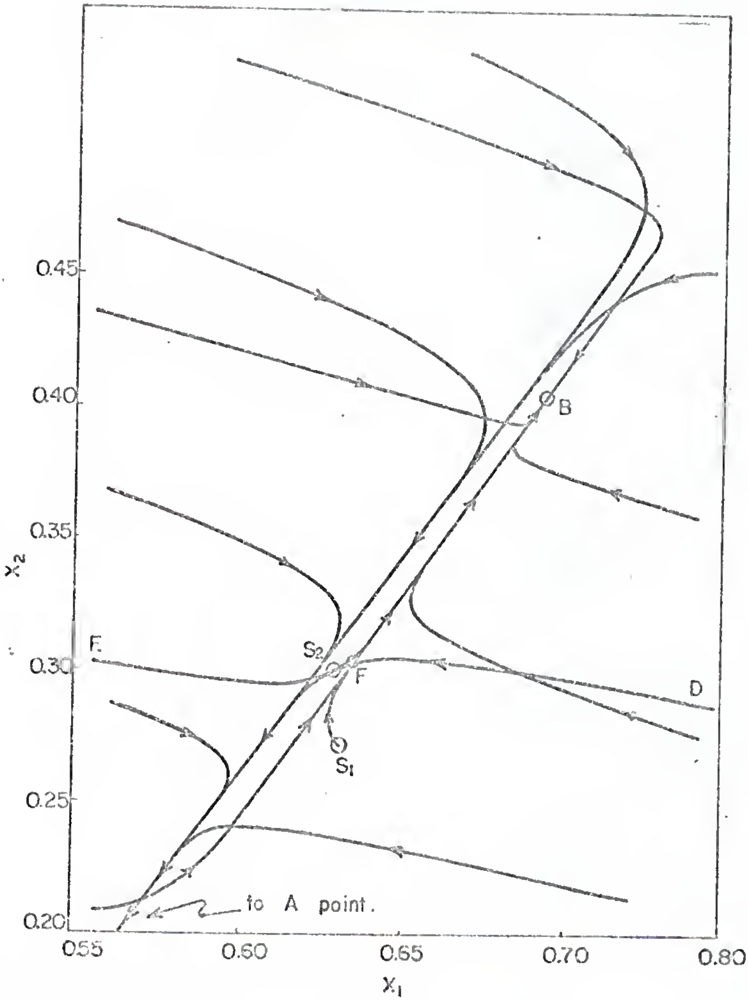


Fig.12. Superimposition of L_{max} and L_{min} response phase planes for Case-2. Paths directed to point B are L_{max} response curves and paths directed to point A are L_{min} response curves.

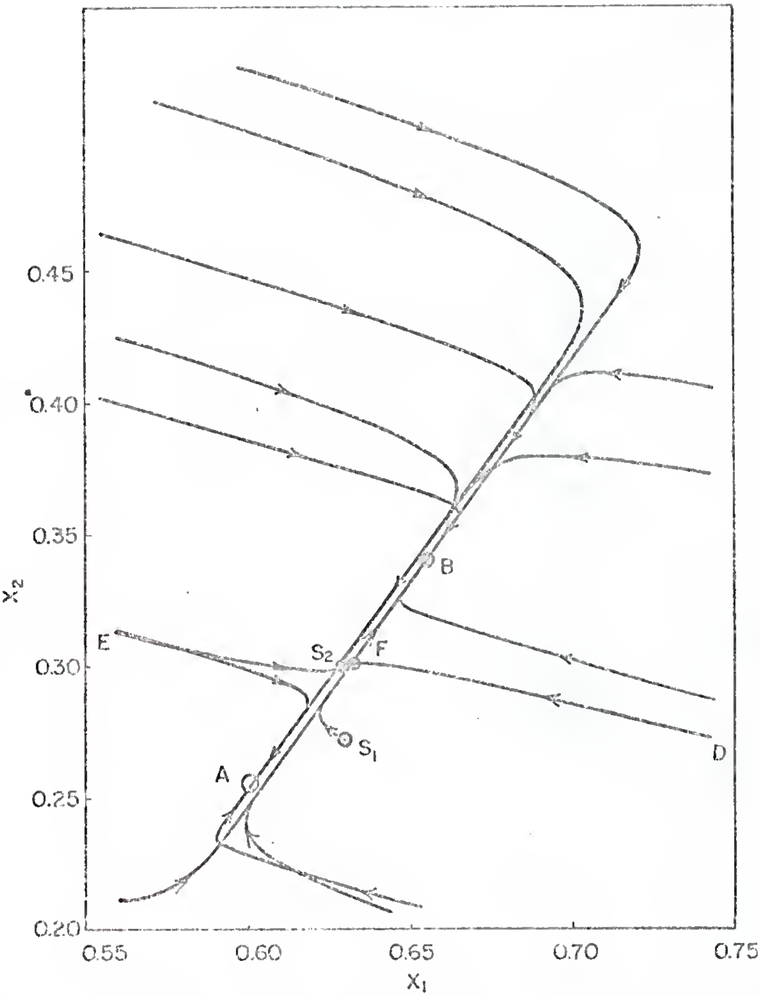


Fig. 13. Superimposition of L_{max} and L_{min} response phase planes for Case 3. Paths directed to point B are L_{max} response curves and paths directed to point A are L_{min} response curves.

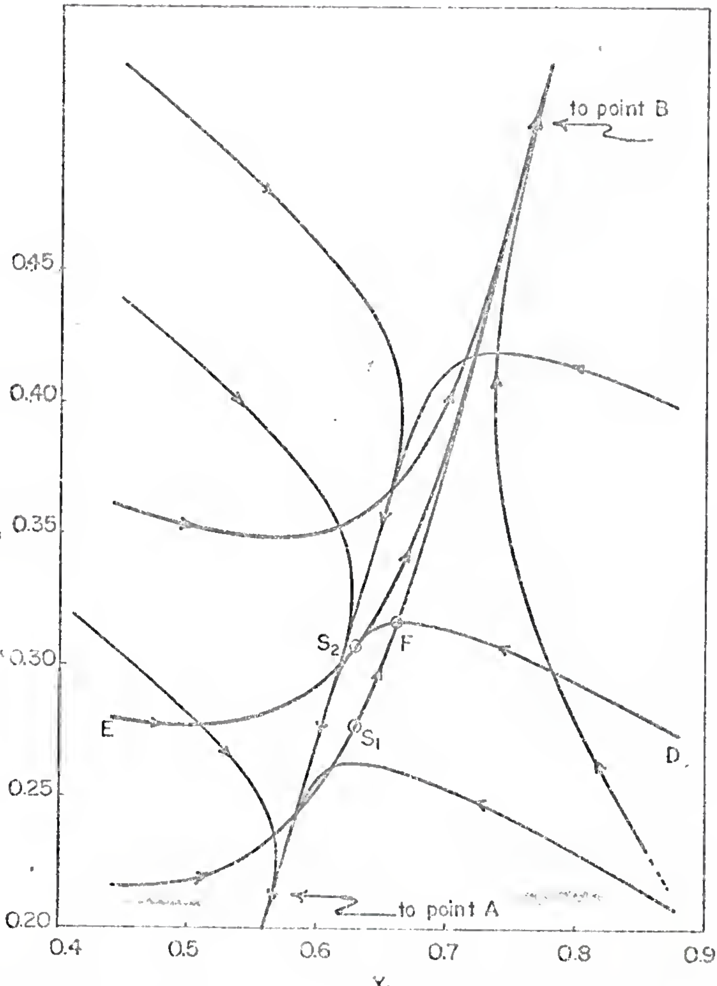


Fig. 14. Superimposition of L_{max} and L_{min} response phase planes for Case 4. Paths directed to point B are L_{max} response curves and paths directed to point A are L_{min} response curves.

reached. The integration was then allowed to proceed with L_{min} until S_2 was reached at which stage the computation was terminated. The value of x_3 at the final state gave the desired minimum of the objective function.

Table 1 shows the results of the above computations as applied to Cases 1, 2, 3 and 4. In each case control starts with L_{max} and switches to L_{min} at the switching time t_s. Figures 15, 16, 17, and 18 show the transient response of the system and the corresponding control policy for Cases 1, 2, 3 and 4.

TABLE 1

RESULTS OF REFERENCE SYSTEM ANALYSIS FOR THE TIME OPTIMAL PROBLEM

	Order in which control is applied	Switching time t_s, min.	Final time T, min
Case 1	$L_{max} = 0.9974$ $L_{min} = 0.833$	2.24	2.80
Case 2	$L_{max} = 0.96452$ $L_{min} = 0.86588$	3.41	4.05
Case 3	$L_{max} = 0.93164$ $L_{min} = 0.89876$	7.63	8.16
Case 4	$L_{max} = 1.333$ $L_{min} = 0.833$	0.56	1.68

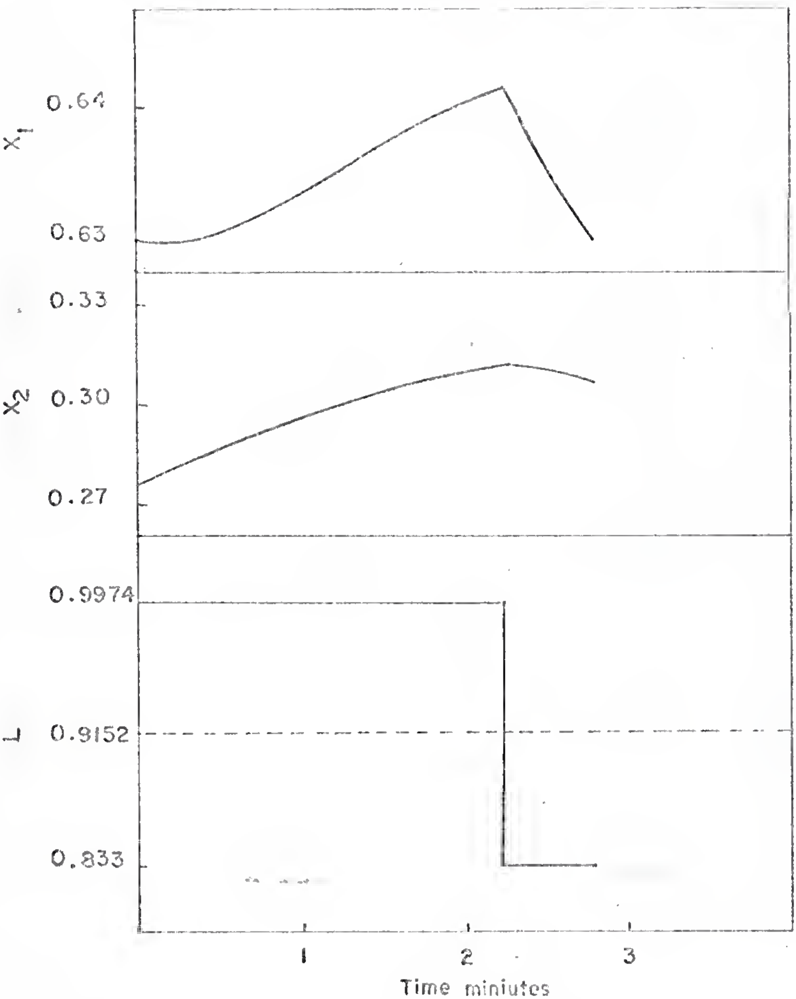


Fig.15. Responses of reference system to bang-bang policy (case I) for time optimal problem (path S_1FS_2 of Fig.11.)

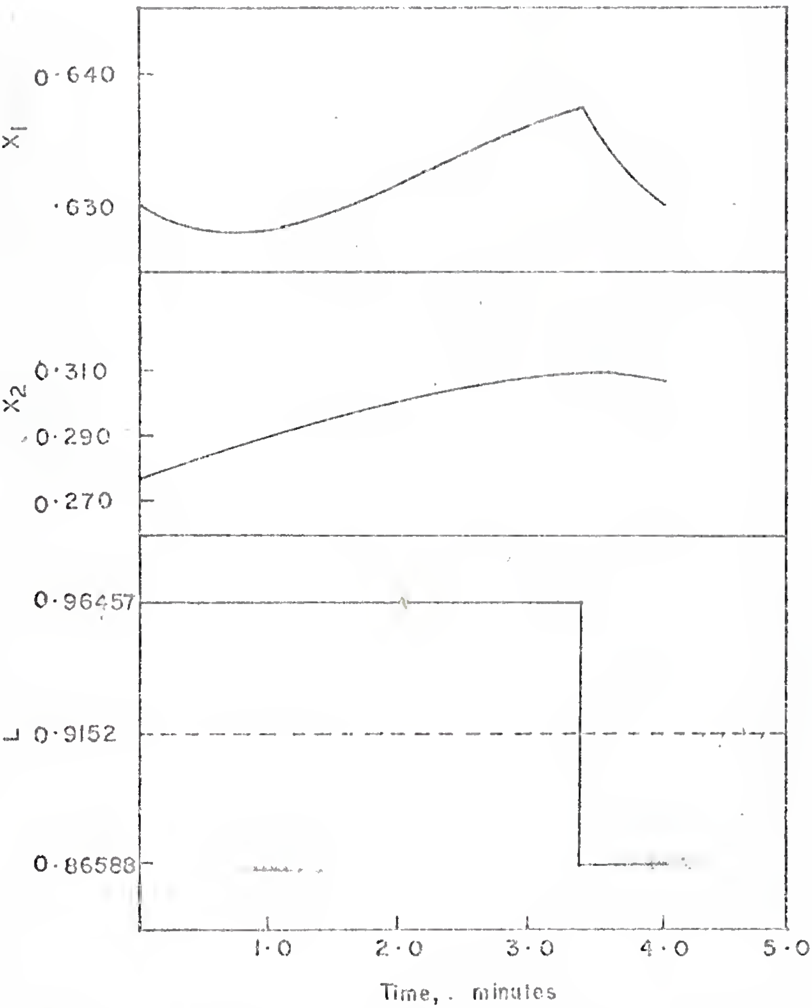


Fig.16. Response of reference system to bang-bang policy(Case.2.) for time optimal problem(path S_1FS_2 of Fig.12.)

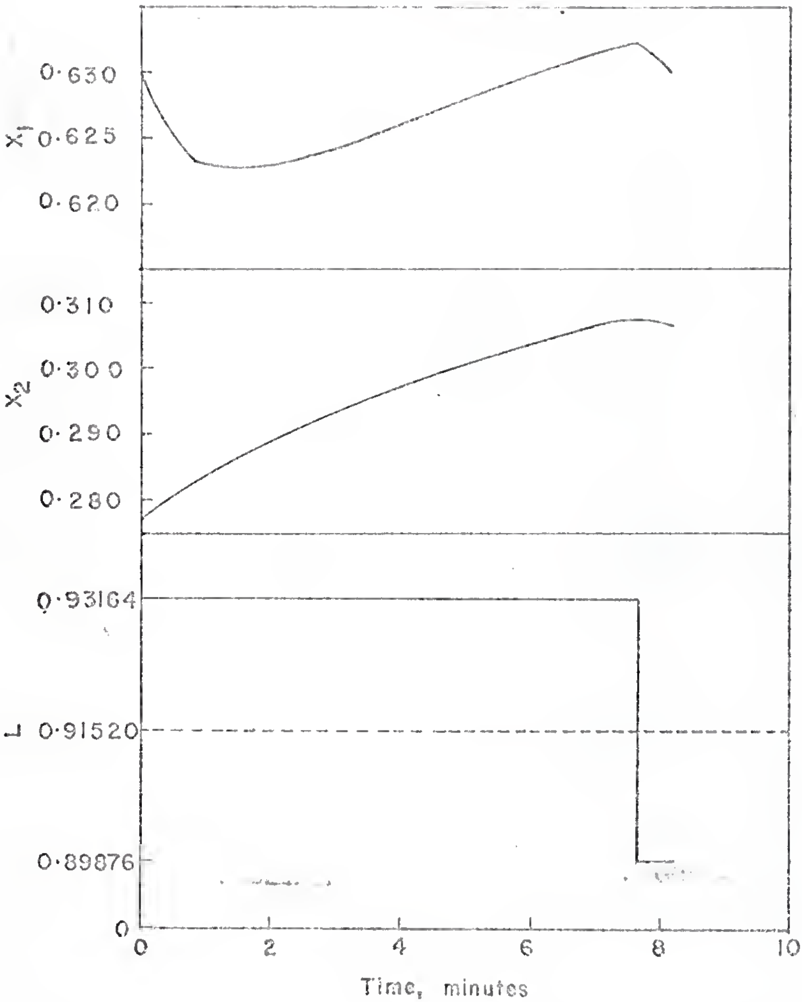


Fig.17. Response of reference system to bang-bang policy (Case 3) for time optimal problem (path S_1FS_2 of Fig.13).

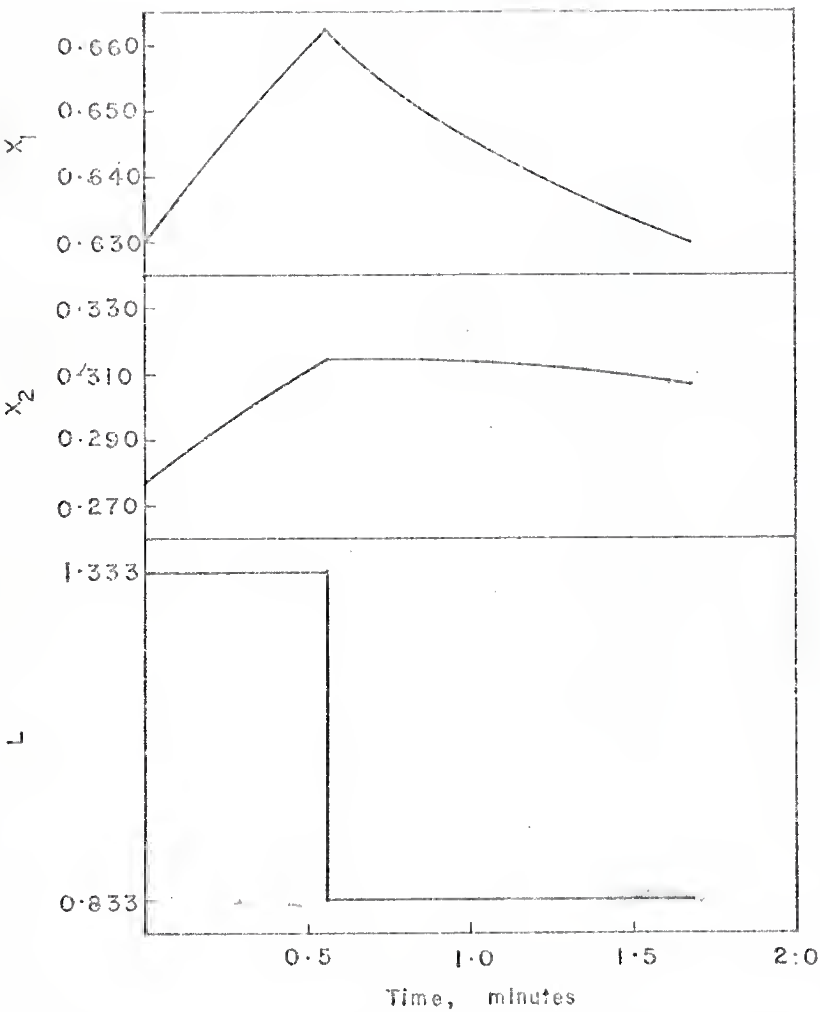


Fig. 18. Response of reference system to bang-bang policy (Case. 4.) for time optimal problem. (Path S_1FS_2 of Fig. 14.).

CHAPTER 3

SYSTEM WITH A TOP TRAY DESCRIBED BY THE MIXING POOL MODEL WITH TWO TANKS IN SERIES

In this chapter we shall consider the same problem as in the previous chapter, i.e., the time optimal problem, except that the top tray of the column will be described by the mixing pool model with two tanks in series; henceforth referred to as the TTIS system.

1. DEVELOPMENT OF PERFORMANCE EQUATIONS

The following assumptions and column characteristics will be appended to those already made in Chapter 2.

(a) The top tray is described by a mixing pool model with two completely mixed pools of equal volume in series.

(b) The vapor rising from the bottom tray is assumed to divide in half before entering each pool of the top tray and likewise after emerging from each pool, the vapor streams merge into a single stream before being totally condensed.

(c) The overhead liquid composition is equal to the mean of the compositions of the vapor streams emerging from the two pools i.e.

$$x_D = \frac{1}{2}(y_1 + y_2) \tag{23}$$

Figure 19 shows a block diagram of the mixing pool model system with the various flow streams involved.

The dynamic behavior of the column in the transient state

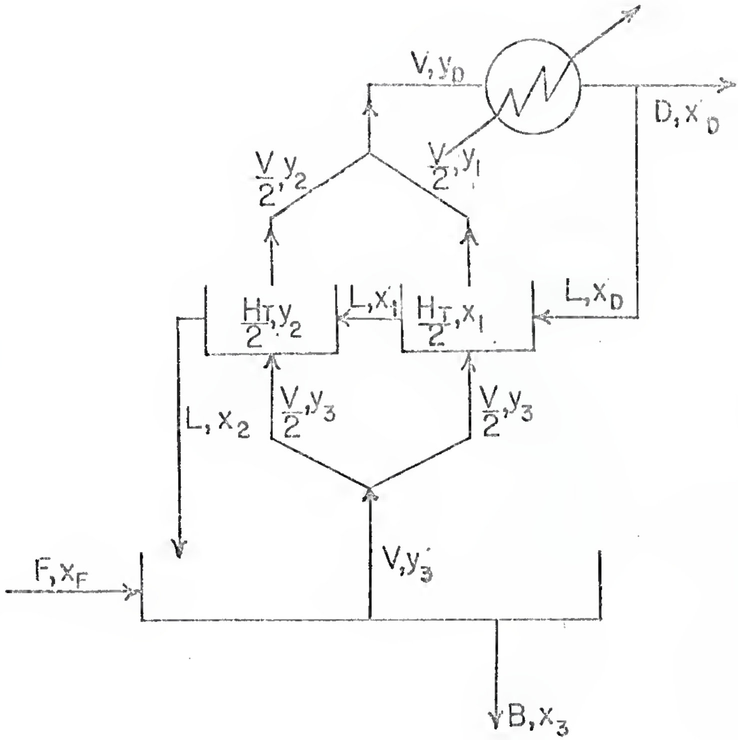


Fig.19. Distillation column with top tray described by mixing pool model with two tanks in series.

may now be written in the differential form by performing a mass balance on each tray along with overall material and light component balances, as follows (see Figures 20, 21, and 22):

For the top tray pool 1,

Input - Output = Accumulation

$$Lx_D + \frac{V}{2} y_3 - Lx_1 - \frac{V}{2} y_1 = \frac{H_T}{2} \frac{dx_1}{dt}$$

Substituting from equation (23) gives

$$\frac{V}{2}(y_1 + y_2) + \frac{V}{2} y_3 - Lx_1 - \frac{V}{2} y_1 = \frac{H_T}{2} \frac{dx_1}{dt}$$

Also since

$$y_i = mx_i + c , \qquad i = 1, 2, 3,$$

we have

$$\frac{L}{2}(mx_1 + c + mx_2 + c) + \frac{V}{2}(mx_3 + c) - Lx_1 - \frac{V}{2}(mx_1 + c)$$
$$= \frac{H_T}{2} \frac{dx_1}{dt}$$

and finally rearranging gives

$$\frac{dx_1}{dt} = \frac{(Lm - 2L - Vm)}{H_T} x_1 + \frac{Lm}{H_T}x_2 + \frac{Vm}{H_T}x_3 + \frac{2Lc}{H_T} \tag{24}$$

For the top tray pool 2,

$$Lx_1 + \frac{V}{2} y_3 - Lx_2 - \frac{V}{2} y_2 = \frac{H_T}{2} \frac{dx_2}{dt}$$

Since

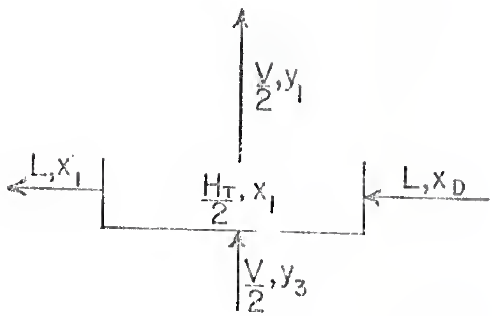


Fig. 20. Material balance streams for pool I of the top tray.

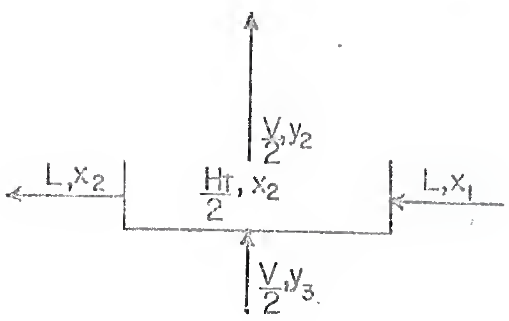


Fig.21 Material balance streams for pool 2 of the top tray.

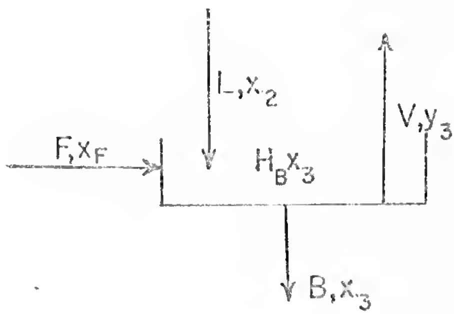


Fig.22 Material balance streams for the bottom tray.

$$y_i = mx_i + c \,, \qquad i = 1,\, 2,\, 3,$$

we have

$$Lx_1 + \frac{V}{2}(mx_3 + c) - Lx_2 - \frac{V}{2}(mx_2 + c) = \frac{H_T}{2}\frac{dx_2}{dt}$$

which on rearrangment yields

$$\frac{dx_2}{dt} = \frac{2L}{H_T}\,x_1 - \frac{(Vm + 2L)}{H_T}\,x_2 + \frac{Vm}{H_T}x_3 \tag{25}$$

And for the bottom tray,

$$Fx_F + Lx_2 - Vy_3 - Bx_3 = H_B\,\frac{dx_3}{dt}$$

Since

$$y_3 = mx_3 + c,$$

we have

$$Fx_F + Lx_2 - V(mx_3 + c) - Bx_3 = H_B\,\frac{dx_3}{dt}$$

and rearranging yields

$$\frac{dx_3}{dt} = \frac{L}{H_B}\,x_2 - \frac{(Vm + F + L - V)}{H_B}x_3 + \frac{Fx_F}{H_B} - \frac{Vc}{H_B} \tag{26}$$

Equations (24), (25), and (26) are the performance equations of the TTIS system. The various parameter values are identical to those in equation (4) and once more the linear vapor-liquid equilibrium i.e.

$$y_i = 0.44x_i + 0.56 \,, \qquad i = 1,\, 2,\, 3$$

is obeyed. The above performance equations were used for simulation purpose on the analog computer whereby the various phase plane plots and transient responses were obtained. The analog computer circuit diagrams are explained in Appendix A. Also the steady state and limiting case analyses are performed in Appendix B.

2. NATURE OF THE PROBLEM

As in the case of the reference system, equations (24), (25), and (26) were solved simultaneously (after setting the left hand sides equal to zero) to obtained the steady state values of x_1, x_2 and x_3. These were found to be

$$x_1 = 0.71467$$
$$x_2 = 0.60909$$

and

$$x_3 = 0.24899$$

Since

$$\begin{aligned} x_D &= \tfrac{1}{2}(mx_1 + mx_2 + 2c) \\ &= 0.22\,x_1 + 0.22\,x_2 + c, \end{aligned} \qquad (27)$$

we have

$$\begin{aligned} x_D &= 0.22 \times 0.71467 + 0.22 \times 0.60909 + 0.56 \\ &= 0.85123. \end{aligned}$$

Let the initial steady state corresponding to $x_F = 0.65$ be designated $S_1' \equiv (x_1 = .71467,\ x_2 = .24899)$. If x_F is instantaneously increased to $x_F = 0.75$ the transient response given by curve OP in Figure 23 results, showing the displacement

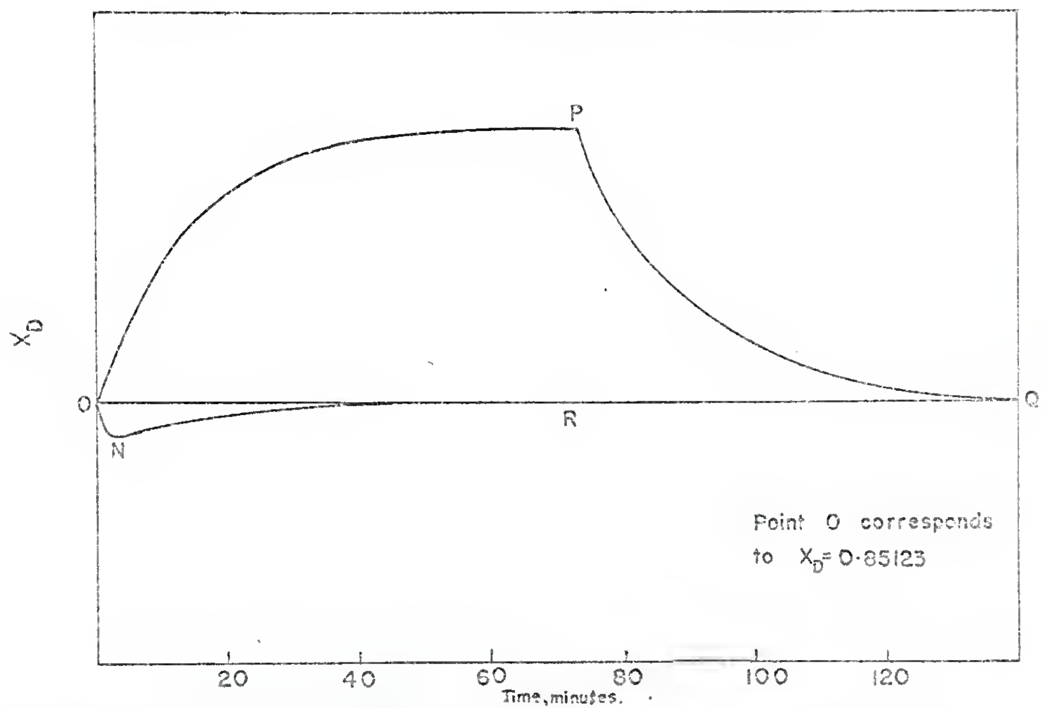


Fig. 23. Displacement and asymptotic restoration of X_D.

of x_D at S_1' to a higher steady state. Once more a value L' of the reflux rate can be computed, which will return x_D to its initial steady state either via PQ or ONR. Such an L' can be determined as follws;

From the overall light component balance, we have

$$Fx_F = Dx_D + Bx_3$$

or

$$x_3 = \frac{Fx_F - Dx_D}{B}$$

$$= \frac{Fx_F - (V-L)x_D}{F + L - V} \tag{28}$$

At steady state equation (24) gives rise to,

$$L = \frac{Vc - Fx_F + Vmx_3 - Vx_3 + Fx_3}{x_2 - x_3} \tag{29}$$

equation (25) to

$$L = \frac{Vmx_2 - Vmx_3}{2(x_1 - x_2)} , \tag{30}$$

and equation (26) to

$$L = \frac{Vmx_1 - Vmx_3}{mx_1 - 2x_1 + mx_2 + 2c} \tag{31}$$

The trial and error procedure for determing L from these four equations is similar to the one used in the case of the reference system i.e. a value for L is assumed and x_3 is calculated from equation (28). Next this value of x_3 is used and L is calculated from each of equations (29), (30), and (31) and checked with the assumed value of L. That value of L which satisfies equations (28), (29), (30), and (31) simultaneously is designated L_1'. The value of L_1' for the TTIS system was found to be 0.922 lb. moles/min., and the steady state resulting from L_1' is $S_2' \equiv$ ($x_1 = 0.71399$, $x_2 = 0.60986$, $x_3 = 0.28247$). Even though L_1' does return x_D to its initial steady state, the time taken to do so is impractical and hence an optimal policy for L has to be determined so as to restore x_D in a time optimal manner. Note: x_D as defined by equation (27) is the same in S_1' and S_2' even though x_1 and x_2 in the two states are different.

3. APPLICATION OF THE MAXIMUM PRINCIPLE ALGORITHM

Once again the optimum reflux policy shall be determined via the Maximum Principle. The performance equations of the system are equations (24), (25), and (26) and are repeated below for convenience.

$$\begin{aligned}
\frac{dx_1}{dt} &= \frac{(Lm - Vm - 2L)}{H_T} x_1 + \frac{Lm}{H_T} x_2 + \frac{Vm}{H_T} x_3 + \frac{2Lc}{H_T} \\
\frac{dx_2}{dt} &= \frac{2L}{H_T} x_1 - \frac{(2L + Vm)}{H_T} x_2 + \frac{Vm}{H_T} x_3 \qquad\qquad (32) \\
\frac{dx_3}{dt} &= \frac{L}{H_B} x_2 - \frac{(Vm + F + L - V)}{H_B} x_3 + \frac{Fx_F - V}{H_B}
\end{aligned}$$

The system is to be transferred from an initial state $S_1' \equiv$ ($x_1 = 0.71467$, $x_2 = 0.60909$, $x_3 = 0.24899$) to the terminal state $S_2' \equiv$ ($x_1 = 0.71399$, $x_2 = 0.60986$, $x_3 = 0.28247$) by manipulating the reflux rate L and simultaneously minimizing the objective function

$$S = \int_{o}^{T} dt \tag{33}$$

where T is unspecified. The control variable is constrained by

$$L_{min} \leq L \leq L_{max} \tag{34}$$

An additional state variable is defined such that

$$x_4(T) = S = \int_{o}^{T} dt \tag{35}$$

thus

$$\frac{dx_4}{dt} = 1$$

According to equation (C-8), the Hamiltonian for this system becomes

$$H = \frac{(Lm - Vm - 2L)}{H_T} x_1 z_1 + \frac{Lm}{H_T} x_2 z_1 + \frac{Vm}{H_T} x_3 z_1 + \frac{2Lc}{H_T} z_1 + \frac{2L}{H_T} x_1 z_2 - \frac{(2L + Vm)}{H_T} x_2 z_2 + \frac{Vm}{H_T} x_3 z_2 + \frac{L}{H_B} x_2 z_3 - \frac{(Vm + F + L - V)}{H_B} x_3 z_3 + \left(\frac{Fx_F - Vc}{H_B}\right) z_3 + z_4 \tag{36}$$

and the adjoint differential system, according to equation (C-9), becomes

$$\frac{dz_1}{dt} = - \frac{(Lm - Vm - 2L)}{H_T} z_1 - \frac{2L}{H_T} z_2 \tag{37}$$

$$\frac{dz_2}{dt} = -\frac{Lm}{H_T} z_1 + \frac{(2L + Vm)}{H_T} z_2 - \frac{L}{H_B} z_3 \tag{38}$$

$$\frac{dz_3}{dt} = -\frac{Vm}{H_T} z_1 - \frac{Vm}{H_T} z_2 + \left(\frac{Vm + F + L - V}{H_B}\right) z_3 \tag{39}$$

$$\frac{dz_4}{dt} = 0 \tag{40}$$

The boundary conditions on the adjoint equations are

$$\begin{array}{ll} z_1(0) \text{ unspecified} & z_1(T) \text{ unspecified} \\ z_2(0) \text{ unspecified} & z_2(T) \text{ unspecified} \\ z_3(0) \text{ unspecified} & z_3(T) \text{ unspecified} \\ z_4(0) \text{ unspecified} & z_4(T) = 1 \end{array} \tag{41}$$

From the final condition on $z_4(t)$ and equation (40), we obtain

$$z_4 = 1, \qquad 0 \leq t \leq T \tag{42}$$

Since the final time T is unspecified and the top tray hold up H_T, is unity, the minimum of the Hamiltonian may be rewritten as

$$\begin{aligned} \min\ H = (&mx_1z_1 - 2x_1z_1 + mx_2z_1 + 2cz_1 + 2x_1z_2 - 2x_2z_2 \\ &+ \frac{x_2z_3}{H_B} - \frac{x_3z_3}{H_B})L + Vmx_3z_1 - Vmx_1z_1 + Vmx_2z_2 - Vmx_3z_2 \\ &- \frac{Vmx_3z_3}{H_B} - \frac{(F - V)}{H_B}x_3z_3 + \left(\frac{Fx_F - Vc}{H_B}\right)z_3 + 1 = 0 \end{aligned} \tag{43}$$

Once more the Hamiltonian is shown linear in the control variable L which implies that the optimal control policy is probably a bang-bang policy as in the case of the reference system. The control policy will be governed by the sign of the switching function, i.e.

$$L = L_{max} \text{ if } \left(mx_1z_1 - 2x_1z_1 + mx_2z_1 + 2cz_1 + 2x_1z_2 - 2x_2z_2 + \frac{x_2z_3}{H_B} - \frac{x_3z_3}{H_B}\right) < 0$$

or (44)

$$L = L_{min} \text{ if } \left(mx_1z_1 - 2x_1z_1 + mx_2z_1 + 2cz_1 + 2x_1z_2 - 2x_2z_2 + \frac{x_2z_3}{H_B} - \frac{x_3z_3}{H_B}\right) > 0$$

Now it is required that the system of equations (32) and (35) be integrated simultaneously with the adjoint system, equations (37), (38) and (39), such that the two point boundary conditions

$x_1(0) = 0.71467$	$x_1(T) = 0.71399$
$x_2(0) = 0.60909$	$x_2(T) = 0.60986$
$x_3(0) = 0.24899$	$x_3(T) = 0.28247$
$x_4(0) = 0.0$	$x_4(T)$ unspecified
$z_1(0) =$ unspecified	$z_1(T)$ unspecified
$z_2(0) =$ unspecified	$z_2(T)$ unspecified
$z_3(0) =$ unspecified	$z_3(T)$ unspecified

are satisfied and the resulting control minimizes the Hamiltonian at every point of its response. Once again the final time is unspecified and hence the minimum value of the Hamiltonian is zero throughout the optimal response.

4. COMPUTATIONAL PROCEDURES

The direct numerical solution of the above set of differential equations is considerably more difficult than that of the reference system since the present solution involves the guessing of two of three initial values $z_1(0)$, $z_2(0)$ and $z_3(0)$ instead of a single initial value as in the case of equation (22). By employing the property that the Hamiltonian must vanish at very point of the optimal transient response we obtain at the initial point, an expression of the form

$$z_1(0) = -\left[\frac{1+(0.2112L(0)-0.2112)z_2(0)+(0.1441L(0)-0.1241)z_3(0)}{0.2732L(0) - 0.2732}\right] \tag{45}$$

In order to eliminate the complexities of the two point boundary value problem, the adjoint equations were discarded and once more the phase plane method of analysis was resorted to. However, due to the three dimensional nature of the problem we are confronted with a phase space rather than a phase plane. Hence, a single phase space will be represented by a set of three phase plane diagrams; that is, the phase space of $x_1x_2x_3$ will be spanned by the phase planes x_1x_2, x_2x_3, and x_1x_3. Also the constraints on L, i.e. L_{max} and L_{min} are picked symmetric with respect to the reflux rate which restores the system to the desired final state,

Case 1 $L_{max} = 1{\cdot}0110$ 100 %
$L_{min} = 0{\cdot}8330$ 0 %

Case 2 $L_{max} = 0{\cdot}9754$ 80%
$L_{min} \doteq 0{\cdot}8686$ 20%

Case 3 $L_{max} \doteq 0{\cdot}9398$ 60%
$L_{min} = 0{\cdot}9042$ 40%

Case 4 $L_{max} = 1{\cdot}3330$
$L_{min} = 0{\cdot}8330$

Fig. 24. Physical bounds within which L is constrained for Cases 1,2,3 and 4.

i.e. symmetric to $L = 0.922$ (which was earlier denoted as L_1' from equations (28), (29), (30) and (31). This gives rise to the following three cases (see Figure 24).

Case 1 $\quad L_{min} = 0.833 \quad L_{max} = 1.011$

Case 2 $\quad L_{min} = 0.8686 \quad L_{max} = 0.9754$

Case 3 $\quad L_{min} = 0.9042 \quad L_{max} = 0.9398$

In addition to the above three cases a fourth case was investigated wherein the entire range of L, as determined in Appendix B, was considered. This corresponds to the total length of the horizontal line in Figure 24. For this case we have

Case 4 $\quad L_{min} = 0.833 \quad L_{max} = 1.333$

Please plane diagrams for the above four cases were plotted with the help of an analog computer and are of the type shown in Figures 25, 26, and 27. Which are the phase planes for Case 4 in each of the phase planes the initial state is denoted by S_1' and the desired final state is denoted by S_2'.

Before going into the search for the optimal control policy, the above four cases were simulated on the analog computer and the resulting phase plane plots were examined. An interesting observation was made from studying these phase planes closely. Starting from the initial state at S_1', the system travels along path $S_1'T$ or $S_1'Q$ depending on whether the initial control action is L_{max} or L_{min} respectively. Once the system travels along one of these initial paths, then no matter what combination of L_{max}

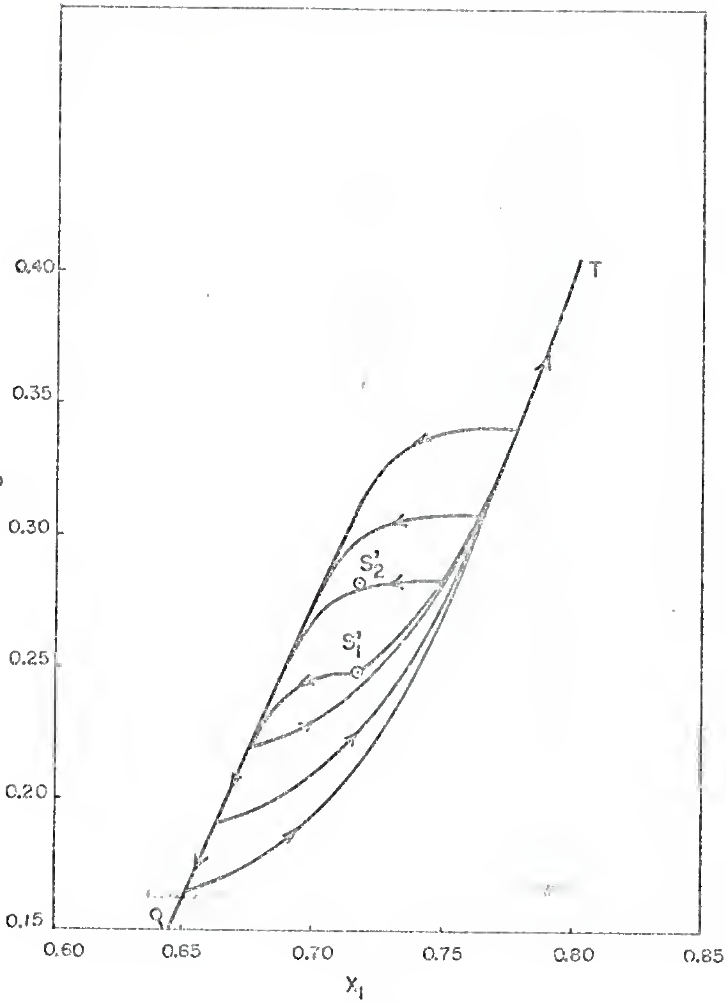


Fig. 25. Superimposed phase planes (x_1, x_3) of two tanks in series system for Case 4. ($L_{max.} = 1{\cdot}333$, $L_{min.} = 0{\cdot}833$).

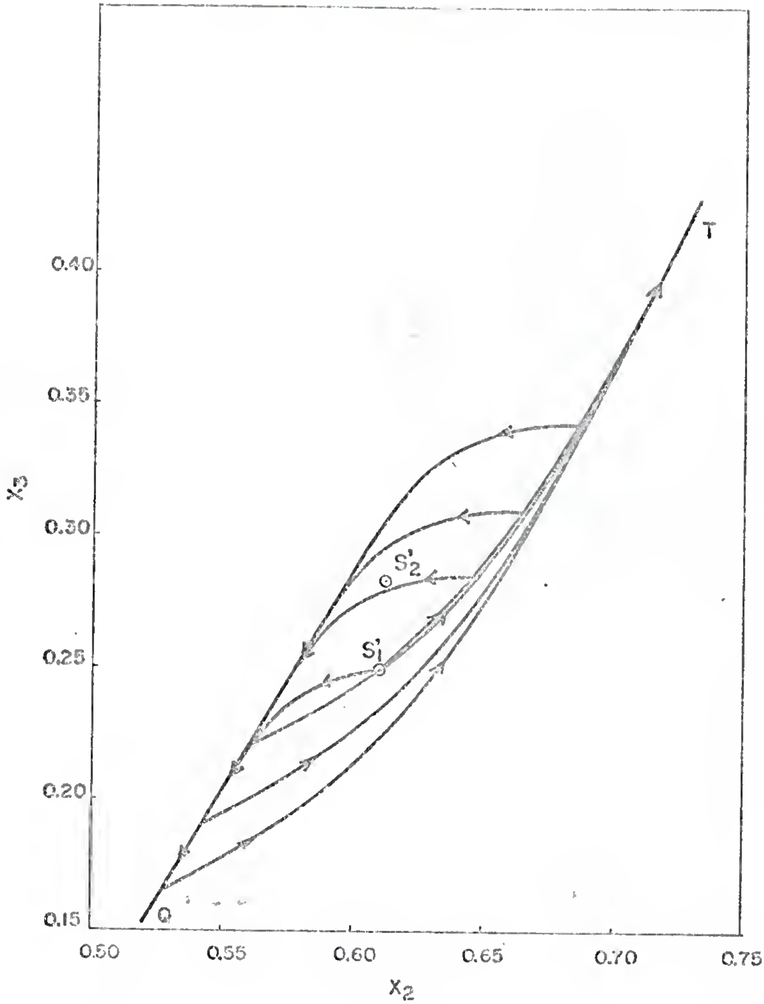


Fig.26. Superimposed phase planes (x_2, x_3) of two tanks in series system for Case 4 ($L_{min} = 0{\cdot}833$, $L_{max} = 1{\cdot}333$).

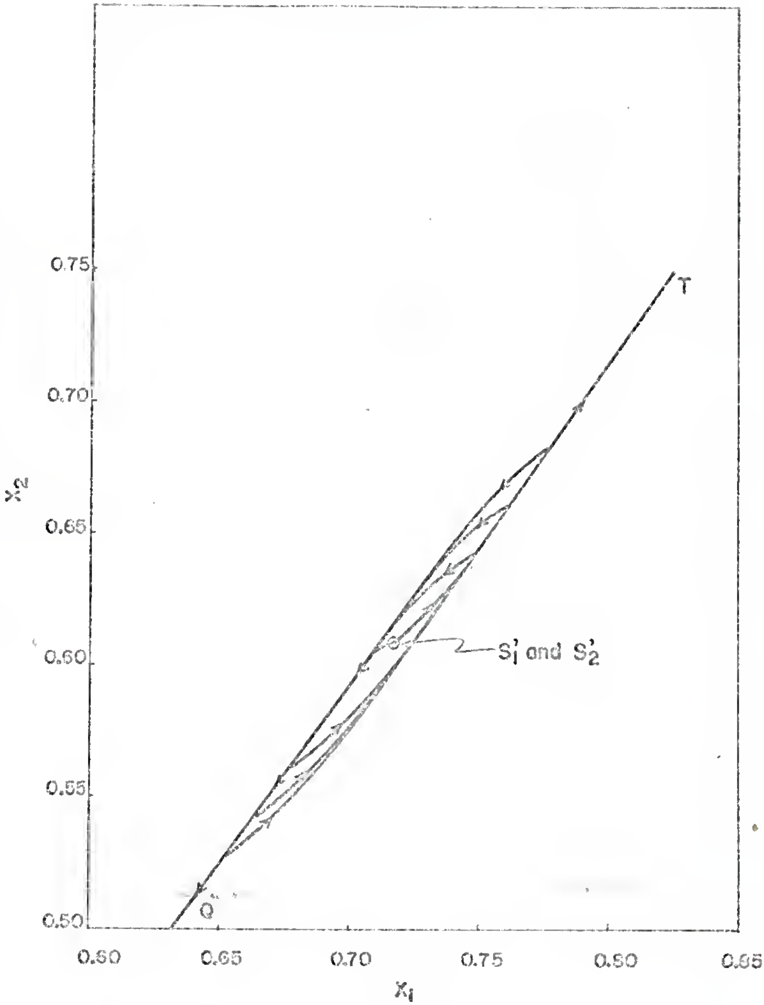


Fig.27. Superimposed phase planes (x_1, x_2) of two tanks in series system for Case 4 (L_{min}=0.833, L_{max}=1.333).

and L_{min} paths is used, the desired final state at S_2' can never be attained. It is essential at this point to explain the fact that even though it may appear from Figures 25, 26 and 27 that a path does exist which passes through S_2', this is not so. In order to elaborate a little on this point let us consider Case 4 whose phase space is represented by the phase planes in Figures 25, 26 and 27. In Figure 25, for instance, it seems obvious that an L_{min} path can pass through S_2', however, on close examination it is found that at S_2' only the final values of x_1 and x_3 are satisfied while x_2 has a value of 0.61476 which is higher than the desired value of 0.60986. Similarly in Figure 26 at S_2' the final values of x_2 and x_3 are satisfied while x_1 is found to be 0.71033 which is lower than the desired value of 0.71399. And likewise in Figure 27 at S_2' the final values of x_1 and x_2 are satisfied while x_3 is found to be considerably lower than the desired value of 0.28247.

The above piece of observation leads to the conclusion that bang-bang control alone cannot achieve the desired terminal state in a finite number of switches. It may be that the terminal state can be attained in an infinite number of bang-bang switches but this being highly impractical, the possibility can be safely abandoned. Therefore, the likelihood of singular or intermediate control becomes a certainty since it seems logical that if the final state cannot be arrived at by purely bang-bang control, some control variable other than L_{max} or L_{min} has to be used in conjunction with L_{max} and L_{min}.

In general, a singular control is indicated whenever the switching function becomes identically zero over one or more positive intervals of time. When such a situation arises the Hamiltonian becomes independent of the control variable and consequently the Maximum Principle fails to yield a well defined control policy. At present there is no generally applicable analytic method by which one can determine, a priori, whether a singular candidate actually represents an optimal trajectory, except in the case of certain restricted classes of problems [12]. Also whenever the singular control is used, the existence theorems of Marcus and Lee [13] does not guarantee the existence of an optimal control policy. A statement of these theorems is given in Appendix C.

Thus the problem of synthesizing the optimal control becomes one of determining the optimal switching hypersurface S which is the union of a bang-bang switching surface S_b and a singular control surface S_s. As an optimal trajectory is traced out in the x, t space, the representative point penetrates the surface S_b at each switch of the bang-bang control given by equation (44). When the optimal control becomes singular, the representative point impinges upon and continues to follow along the surface S_s. A typical situation is illustrated in Figure 28.

In general, the singular trajectories become unstable solutions of the canonical equations, equations (32), (35), (37), (38), (39) and (40), when the bang-bang control as represented by equation (44) is utilized. That is, the control function defined by equation (44) will not cause the representative point to remain along the singular control surface S_s. For this

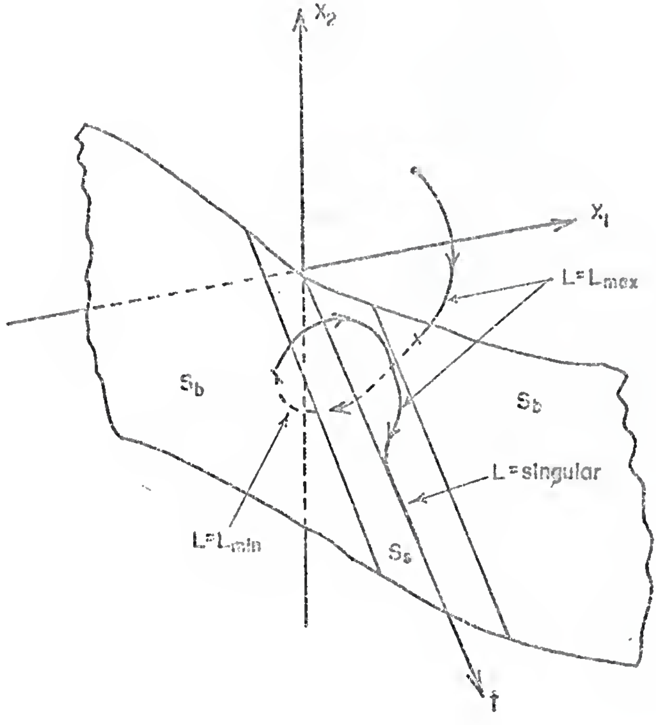


Fig.28. A typical optimal trajectory in x, t space showing singular and nonsingular subarcs [9].

reason, it is easy to overlook singular solutions when ordinary computer searching methods are used to integrate the canonical equations [12]. In principle, the determination of the switching surface S is accomplished by expressing the initial value of the (optimal) adjoint vector z as a function of the initial conditions vector x(0). In practice, this procedure leads to a rather difficult analytic problem which, so far, has been solved in only a few special cases. Nevertheless, if the solution for the optimal control involves subarcs of singular control, then it may be possible (with emphasis on the word "may") to determine z(x, t) on S_s without knowing the general expression for z(x, t), by making use of the fact that on S_s the switching function and all its time derivatives are identically zero [12]. However, this method involves the heaviest of algebraic manipulations even for two dimensional problems, and certainly encumbers the analytic procedure for three dimensional problems such as the present case. Also the fact that in addition to the algebraic manipulations, a certain line integral has to be evaluated, makes the above mode of approach to determining the singular solution quite formidable.

A more direct numerical approach, as outlined by Grethlein and Lapidus [15] in the paper entitled "Time optimal control of non linear systems with constraints", was used to obtain the control policy for the present problem. It should be borne firmly in mind that the physical realizability of singular control situations is not sufficient to establish the optimality of singular control and consequently the control policy as obtained by the method of Grethlein and Lapidus may not be a truely optimal policy but it certainly is one of the methods available for determining suboptimal policies.

The approach taken by Grethlein and Lapidus is to predict, over one sampling period by means of the mathematical process models, the responses for a selected number of control levels. A modified objective function (usually of the least squares form) is defined, and by evaluating this objective function for the predicted values, the optimum control action is selected at each sampling period. It is that control action which minimizes the objective function. The overall control system with its optimizing scheme is called the "optimum predictor-controller".

In general the dynamic description of a process can be represented by a set of first order differential equations written in vector form as

$$\frac{dx(t)}{dt} = \phi[x(t);\ \theta(t)] \tag{46}$$

where x(t) represents the state variables and θ(t) represents the control variables. Thus the state of the process is interpreted as a vector in state space and each state of the process which is different from another has a unique set of coordinates.

In principle the transient behavior is obtained by solving the differential equations simultaneously with the proper initial conditions and control variables. As a result a future state of the process at any time T can be evaluated if some initial state $x(t_0)$ is given in addition to the control vector $\theta(t)$ for all time $t_0 \leq t \leq T$. The existence of a solution does not imply that it is necessarily an analytic solution. In most nonlinear cases only numerical solutions are obtainable.

Since a computer can only operate on digits which represent the state of the process at a discrete point in time, any control system utilizing a digital computer will necessarily be a sampled data system. From the point of view of the controller, a process is represented as a sequence of numbers spaced in time. Similarly the control action is a sequence of numbers. It is convenient to take the time interval between sampling points equal to λ so that real time can be represented at the sampling points by

$$t = \lambda,\ 2\lambda,\ 3\lambda,\ \ldots,\ k\lambda,\ \ldots$$

Although the control and state vectors of the process vary continuously with time, their specific value at the sampling point $t = k\lambda$ is represented by $\theta(k\lambda)$ and $x(k\lambda)$ respectively or more simply by $\theta(k)$ and $x(k)$. If the sampling period is taken small enough so that the control $\theta(t)$ for $k\lambda \leq t \leq (k + 1)\lambda$ can be considered essentially constant and equal to $\theta(k)$ for the entire period, the dynamic equation for the process will become

$$\frac{dx}{dt} = \phi[x;\ \theta(k)] \tag{47}$$

for

$$k\lambda \leq t \leq (k + 1)\lambda.$$

Thus the dynamic behavior of the process can be expressed in the form

$$x(k + 1) = \phi[x(k);\ \theta(k);\ \lambda] \tag{48}$$

With a knowledge of the state of the process and the input vector at any time $t = k$, equation (48) gives the state of the process at the next sampling point.

Before it is possible to single out a particular controller as being optimum, it is necessary to define quantitatively some measure of merit by which the performance of the system is evaluated. The simplest type of measure of performance is some function of the difference between the actual output of a process at a given time and that desired for the dynamic system. A convenient measure may be defined as

$$S(t) = a_1[x_1(t) - x_1^*]^2 + a_2[x_2(t) - x_2^*]^2 + \cdots \tag{49}$$

where a_1, a_2, ... are appropriate weighing factors and x_1^*, x_2^*, ... are the coordinates of the desired final state. Assuming that the control vector is changed only at the sampling point, equation (49) is summed over all time

$$J(N) = \sum_{k=1}^{N} S(k\lambda)\lambda \qquad N \longrightarrow \infty \tag{50}$$

where N is taken sufficiently large to cover the entire transient period. Thus the optimum dynamic response is obtained when a discrete set of control inputs $\theta(k)$ are found such that

$$J^*(N) = \underset{\theta(k)}{\text{Min}} \sum_{k=1}^{N} S(k\lambda) \qquad N \longrightarrow \infty \tag{51}$$

At this stage montion must be made that if the system is table, the dynamic response will ultimately come to an equilibrium or steady state at some $k = N_{equil}$.

The optimum control action at any given sampling period is generated by the following computation scheme. Since the present state of the process $x(k)$ is known as a result of a feedback measurement, the state of the process at the next sampling period $x(k + 1)$ can be calculated from equation (48) for any number of control actions. Specifically, the state of the process is calculated for the maximum control θ_{max}, the minimum control action θ_{min}, and three intermediate control actions θ_1, θ_2 and θ_3; thus

$$\begin{aligned} x^1(k + 1) &= \phi[x(k);\ \theta_{max};\ \lambda] \\ x^2(k + 1) &= \phi[x(k);\ \theta_{min};\ \lambda] \\ x^3(k + 1) &= \phi[x(k);\ \theta_1;\ \lambda] \\ x^4(k + 1) &= \phi[x(k);\ \theta_2;\ \lambda] \\ x^5(k + 1) &= \phi[x(k);\ \theta_3;\ \lambda] \end{aligned} \tag{52}$$

where the superscript numbers are used to distinguish the predicted states. The responses to the various control actions are evaluated with the aid of the objective function for the $(k + 1)$ period, namely

$$P^1(k + 1) = P[x^*;\ x^1(k + 1)] \tag{53}$$

$$P^2(k+1) = P[x^*;\ x^2(k+1)]$$

$$P^3(k+1) = P[x^*;\ x^3(k+1)]$$

$$P^4(k+1) = P[x^*;\ x^4(k+1)] \qquad \text{(53 cont.)}$$

$$P^5(k+1) = P[x^*;\ x^5(k+1)]$$

The possible configurations for the predicted objective function and the control action are shown in Figure 29. The computer routine selects the optimum control action at $t = k\lambda$ on the basis of a predicted minimum objective functions at $t = (k+1)\lambda$. For configuration (a) or (b), θ_{max} is selected as the optimum control action. For configuration (c) or (d), θ_{min} is selected as the optimum control action. The need to predict the performance for some intermediate control action becomes clear when the optimum is not one of the extreme values. When configuration (e), (f) or (g) occurs, the computer fits a second order curve through the minimum point and its two neighboring points already calculated, and finds the minimum in the curve. The corresponding value of θ becomes the optimum control action for that period.

The computer logic flow chart for the above method is shown in Figure 30. The explanation of the various steps in the corresponding numbered boxes in Figure 30 is as follows.

1. The five values of the decision variable are read in, where AL(1) = L_{min} AL(5) = L_{max} and AL(2), AL(3), and AL(4) are three intermediate values of the decision variable L.

2. The lower bound of the first sampling period (PRMT(1)),

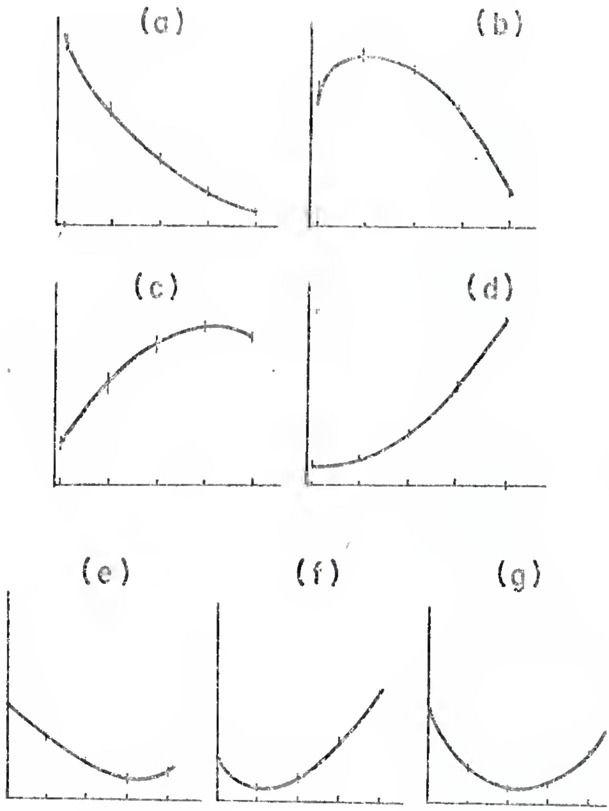


Fig. 29. Possible configurations for predicted performance function.

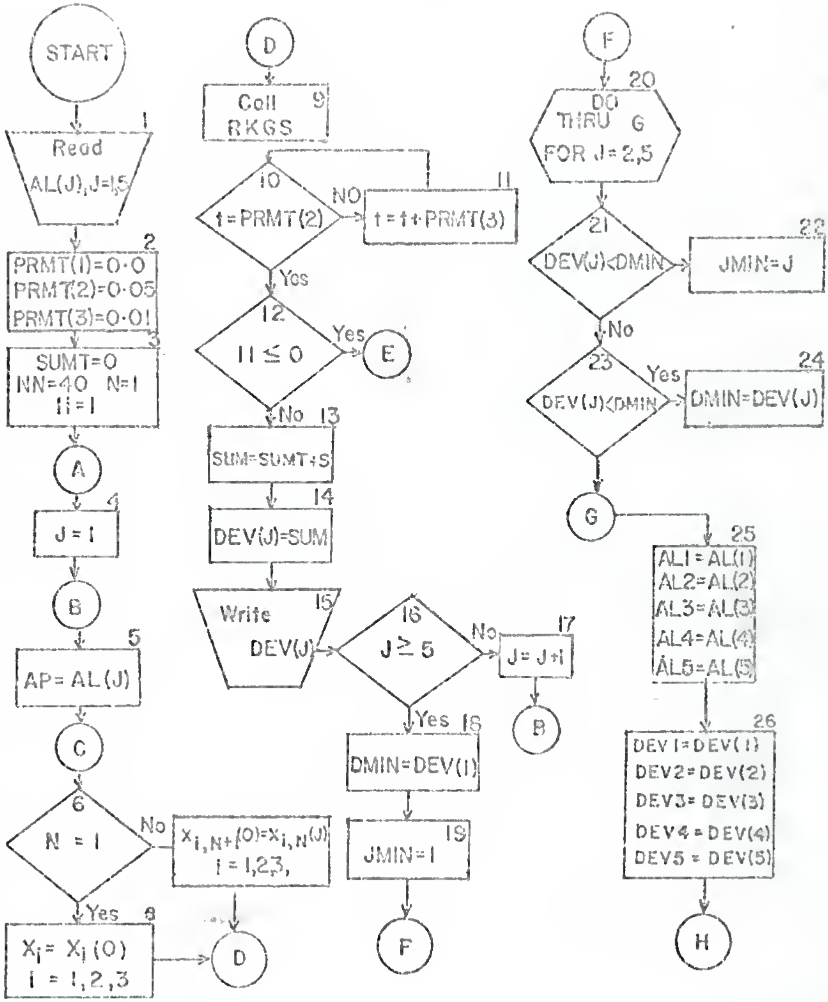
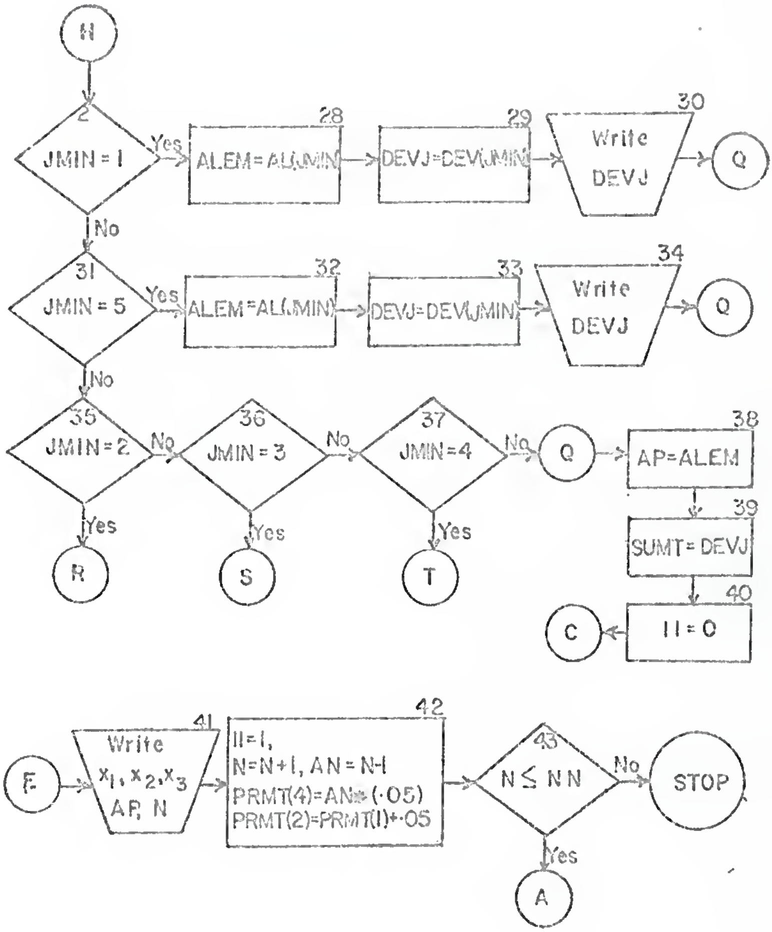


Fig.30. Computer logic flow chart for method of Grethlein and Lapidus.



H
2
JMIN = 1
Yes
No
28
ALEM = AL(JMIN)
29
DEVJ = DEV(JMIN)
30
Write
DEVJ
Q
31
JMIN = 5
Yes
No
32
ALEM = AL(JMIN)
33
DEVJ = DEV(JMIN)
34
Write
DEVJ
Q
35
JMIN = 2
No
Yes
R
36
JMIN = 3
No
Yes
S
37
JMIN = 4
No
Yes
T
Q
38
AP = ALEM
39
SUMT = DEVJ
40
II = 0
C
F
41
Write
x1, x2, x3
AP, N
42
II = I,
N = N + I, AN = N-I
PRMT(4) = AN*(·05)
PRMT(2) = PRMT(I)+·05
43
N ≤ NN
No
STOP
Yes
A

Fig.30. (cont.)

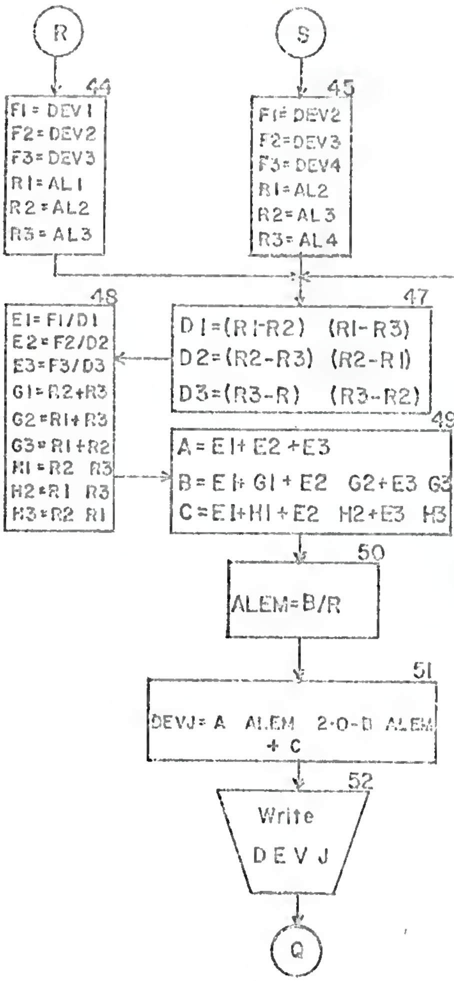

R
S
T
44
FI = DEV I
F2 = DEV2
F3 = DEV3
R I = AL I
R 2 = AL2
R3 = AL3
45
FI = DEV2
F2 = DEV3
F3 = DEV4
R I = AL2
R2 = AL 3
R3 = AL 4
46
FI = DEV3
F2 = DEV4
F3 = DEV5
R I = AL3
R2 = AL4
R3 = AL5
48
EI = FI/DI
E2 = F2/D2
E3 = F3/D3
GI = R2+R3
G2 = RI+R3
G3 = RI+R2
HI = R2 R3
H2 = RI R3
H3 = R2 RI
47
D I = (R I-R2) (RI-R3)
D2 = (R2-R3) (R2-R I)
D3 = (R3-R) (R3-R2)
49
A = E I + E2 + E3
B = E I + GI + E2 G2 + E3 G3
C = E I + HI + E2 H2 + E3 H3
50
ALEM = B/R
51
DEVJ = A ALEM 2·0-D ALEM + C
52
Write DEV J
Q

Fig.30.(Cont.)

the upper bound of the first sampling period (PRMT(2)), and the integrating increment (PRMT(3)) are initialized.

3. The number of sampling periods (NN), the current sampling period (N), and the initial minimum deviation (SUMT) are initialized. The switch II is set equal to unity. (II can be either 1 or 0).

4. The subscript J is initialized.

5. The decision variable (AP) is initialized.

6-8. The current value of the sampling period is checked and accordingly the initial values of each sampling period are specified. For N = 1, the initial values are specified in Box 8. For N > 1, the initial values are specified in box 7 wherein the terminated state of the Nth sampling period becomes the initial state of the (N+1)th sampling period.

9. Subroutine RKGS is called and the integration commences.

10, 11. The extent of the integration is checked to see whether the upper bound of the current sampling period has been reached if so, command transfers to box 12, and if not, command passes to box 11 where the time is incremented and the integration proceeds.

12. The value of the switch II is checked. If II = 1, command transfers to box 13; otherwise to box 41.

13. The quantity SUM is defined as the minimum deviation up to the (N-1)th sampling period (SUMT) plus the current deviation (S).

14. The variable DEV(J) is set equal to SUM and this represents the total deviation corresponding to the current value

of J.

15. DEV(J) is written out.

16, 17. The subscript J is checked to make sure all the 5 decision variables defined in box 1 have been used. If J is less than 5, it is incremented by unity and command is passed to box 5. If J is equal to 5 command passes to box 18.

18-24. The minimum of the five DEV(J) is determined, and the value of J corresponding to the minimum DEV(J) is stored as JMIN.

25, 26. The new variables AL1 to AL5 and DEV1 to DEV5 are defined.

27-30. If JMIN = 1, then ALEM is defined as the decision variable corresponding to JMIN and DEVJ is defined as the deviation corresponding to JMIN. DEVJ is written out and command is transferred to box 38.

31-34. If JMIN = 5, then ALEM is defined as the decision variable corresponding to JMIN and DEVJ is defined as the deviation corresponding to JMIN. DEVJ is written out and command is transferred to box 38.

35-37. If JMIN = 2, 3, or 4, command is transferred to box 44, 45 or 46 respectively whereby a second order curve will be fitted as shown in Figure 29 (e), (f) and (g) and the minimum of the curve determined.

38. The decision variable is set equal to the minimizing decision variable as determined from boxes 28, 29, or 50.

39. SUMT is set equal to DEVJ as the minimum total deviation up to the present sampling period.

40. The switch II is set equal to zero and command is transferred to box 6. The reason for setting II = 0 is that once the minimizing decision variable has been determined then the computer can skip all the command from boxes 13 to 40 inclusive, thereby command being transferred from box 12 to box 41.

41. The values of the state variables x_1, x_2 and x_3 are written out along with the minimizing decision variable and the number of the current sampling period.

42. Herein are initialized the various parameters for the next sampling period and II is again set equal to 1.

43. If the number of the new sampling period has not exceeded the value of NN then command is transferred to box 4 and the above procedure repeated. If the number of the new sampling period exceeds NN, the computation is terminated.

44-49. The coefficients of a second order polynomial through three points are calculated. The polynomial is of the form $y = ax^2 - bx + c$ where y corresponds to the deviation and x corresponds to the decision variable.

50. The minimizing decision variable is determined by setting $\frac{dy}{dx} = 0$, i.e. $2ax - b = 0$, $x = b/2a$.

51. From the minimizing decision variable, the corresponding minimum deviation is determined.

52. The minimum deviation DEVJ is written out and command is transferred to box 38.

The above method was applied to Cases 1, 2, 3 and 4 and the optimal (or suboptimal) policy was obtained in each case. In order that the method be applicable to our problem a few changes were incorporated; namely the control action was selected so that the dynamic response would minimize an objective function of the type given in equation (49) rathers than the original form in equation (33). Since in the present example concentrations are being controlled a suitable overall objective function would be that defined by

$$J(N) = \sum_{k=1}^{N} S(k)\lambda$$

with

$$S(k) = a[x_1(k) - x_1^*]^2 + b[x_2(k) - x_2^*]^2 + c[x_3(k) - x_3^*]^2 \tag{54}$$

where x_1^*, x_2^*, and x_3^* are the coordinates of the desired final state $S_2' \equiv (x_1 = 0.71399,\ x_2 = 0.60986,\ x_3 = 0.28247)$, and a, b, and c are appropriate weighting factors. According to Grethlein and Lapidus [15] there is no prior way of determining the exact weights, but the dynamic properties of the system can serve as a guide line. In our particular problem the system is to be transferred from an initial state $S_1' \equiv (x_1 = 0.71467,\ x_2 = 0.60909,\ x_3 = 0.24899)$ to the terminal state $S_2' \equiv (x_1 = 0.71399,\ x_2 = 0.60986,\ x_3 = 0.28247)$ in a time optimal manner. Comparing S_1' and S_2' we see that x_1 and x_2 don't have as much distance to cover in the state space as x_3 does and consequently we weigh the deviation of x_3 more heavily that the deviation of

x_1 and x_2. The rationale for doing this is that in view of the larger margin of operation in x_3 and hence a larger margin for its deviation, we penalize it heavily thus making sure that it attains the desired final state without undue deviation. Thus the control action is biased mainly towards the deviation of x_3. In making x_3 attain its desired final state in the most direct manner we also ensure that x_1 and x_2 attain their desired final states since x_1, x_2, and x_3 are interrelated by material balances and also the system dynamics are based on these material balances.

The predictor controller that is used along with an objective function of the type in equation (54), makes certain that the system attains the final state S_2' for a wide range of values of the weighting factors a, b and c. However since we're interested in time optimality we must select a, b and c such that S_2' is attained in the shortest possible time.

In experimenting with the above controller it was found that the response time τ in going from S_1' to S_2' was significantly decreased as the ratio of c:a and c:b was increased. Thus the weighting factors were picked such that a and b are equal and the ratio c:a or c:b is an integral power of 10.

The scheme used for selecting the optimal values of a, b and c is as follows:

1. Given the initial state S_1' the optimal predictor controller was utilized so as to minimize the objective function in equation (54) with ratio of weighting factors c:a = c:b = 10.

2. The time at which the desired state S_2' is attained

is noted as τ_1.

3. The procedure in step 1 is repeated with c:a = c:b = 10^i for i = 2, 3, ... and the time at which state S_2' is attained is noted as τ_i, i = 2, 3, ...

The above listing of τ_i gives the times required to transfer the system form state S_1' to the state S_2' for increasing values of the ratios c:a or c:b. It was found that as i increases τ_i decreases and that there is a certain i beyond which any further increase in i does not produce any decrease in τ_i. This is the i that determines the optimal ratio c:a = c:b = 10^i. These values of a, b and c and the corresponding control policy which transfers the system from S_1' to S_2' was then accepted as the optimum predictor controller achieving time optimality. The value of i and hence the values of a, b and c are found to vary as we go from Case 1 to Case 4.

Hence in recapitulating we must realize that the original objective function in equation (33) which demands time optimality has been discarded and in its place a modified objective function of the type in equation (49) is adopted. The weighting factors in equation (49) are then experimented with so that the system is transferred from the state S_1' to the state S_2' in the most direct way and in a time optimal manner.

The optimal response for the four cases is shown in Figures 31, 32, 33, and 34. Basically two types of control policies are encountered. The first type (in cases 1, 2 and 3) wherein initially L_{max} is used until the first switch after which singular control is used finally ending up asymptotically at L_1'.

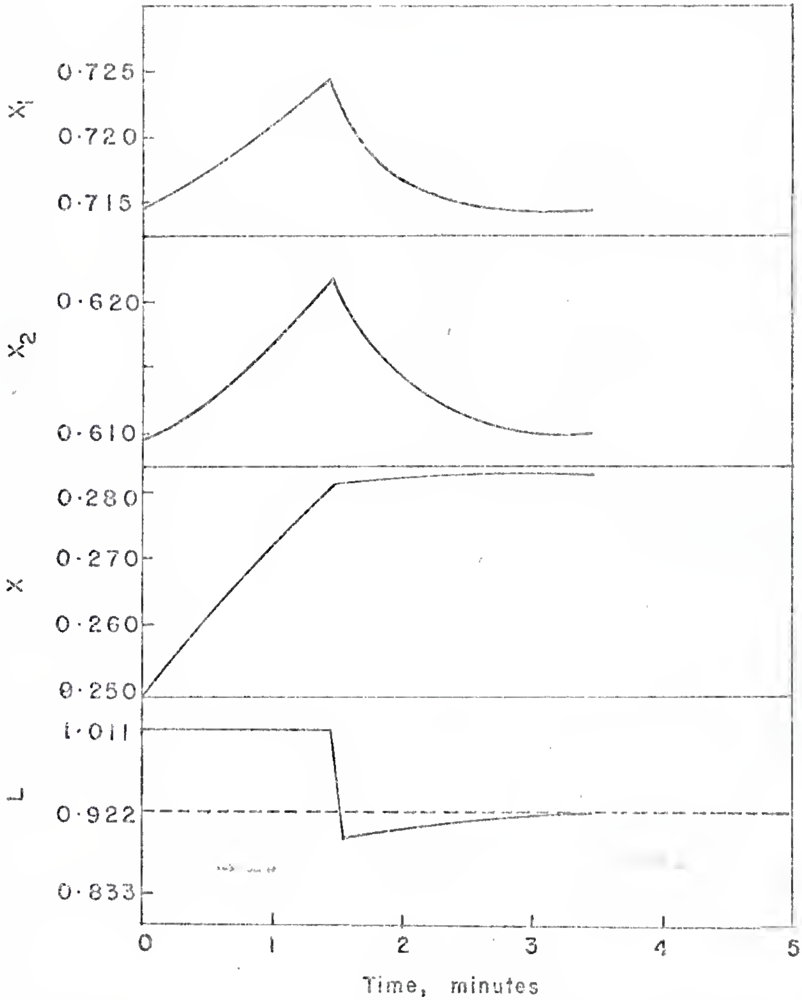


Fig.31. Response of the two tanks in series system to singular control (Case I) for time optimal problem.

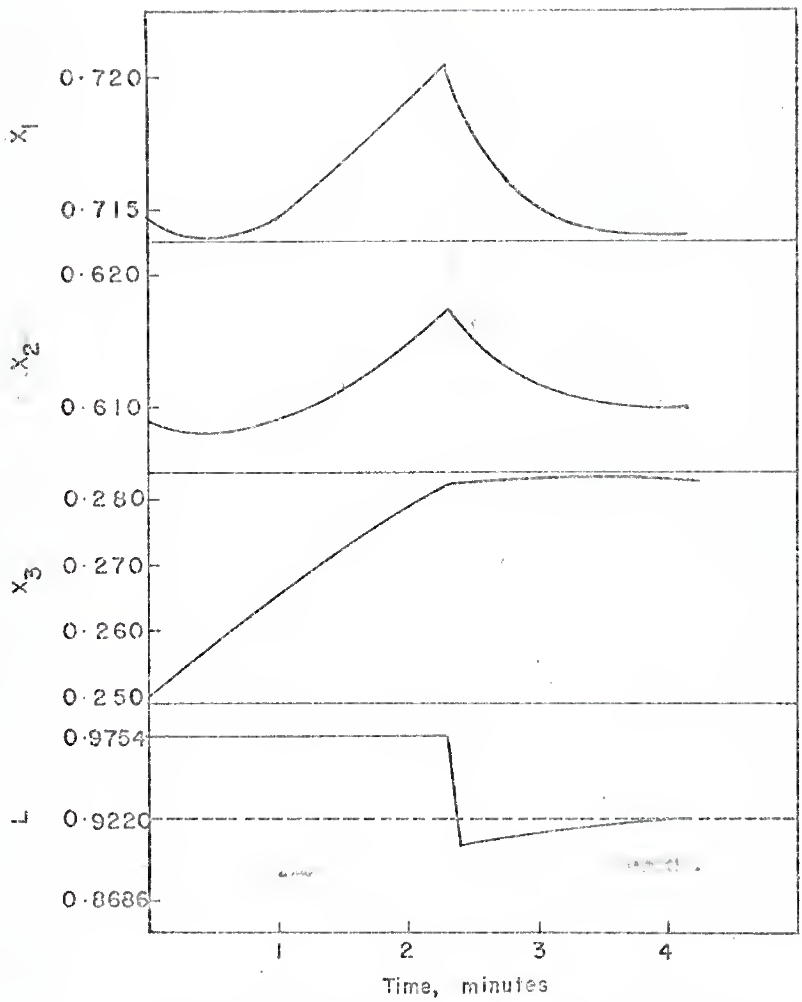


Fig.32. Response of the two tanks in series system to singular control (Case.2.) for time optimal problem.

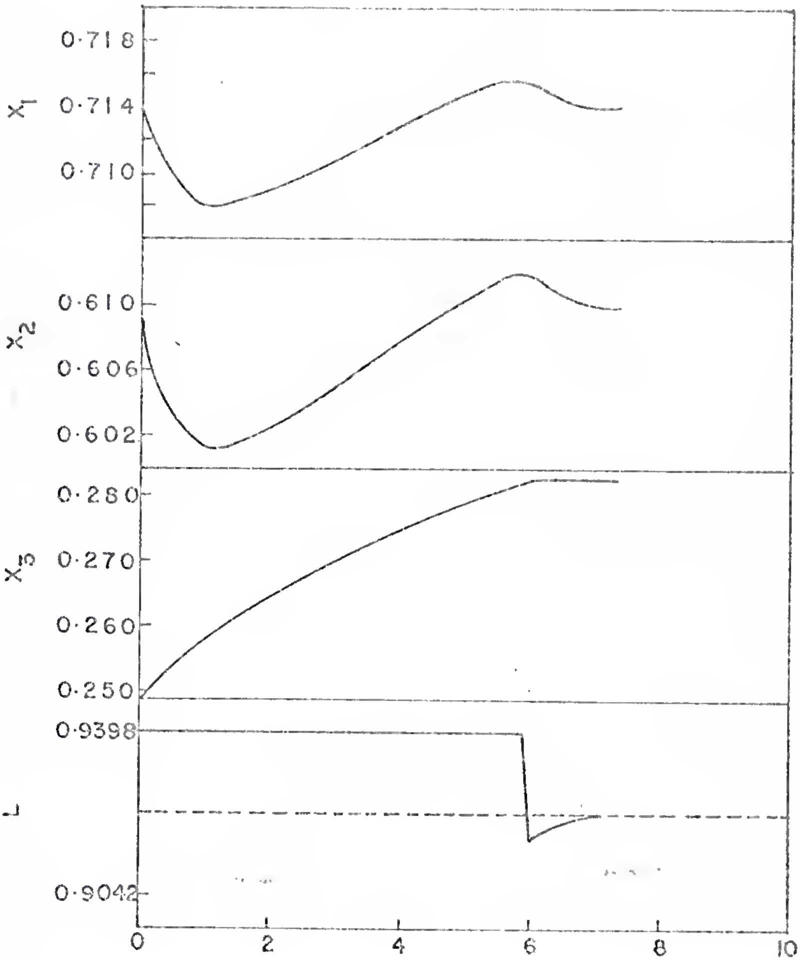


Fig.33. Response of the two tanks in series system singular control (Case 3) for time optimal problem.

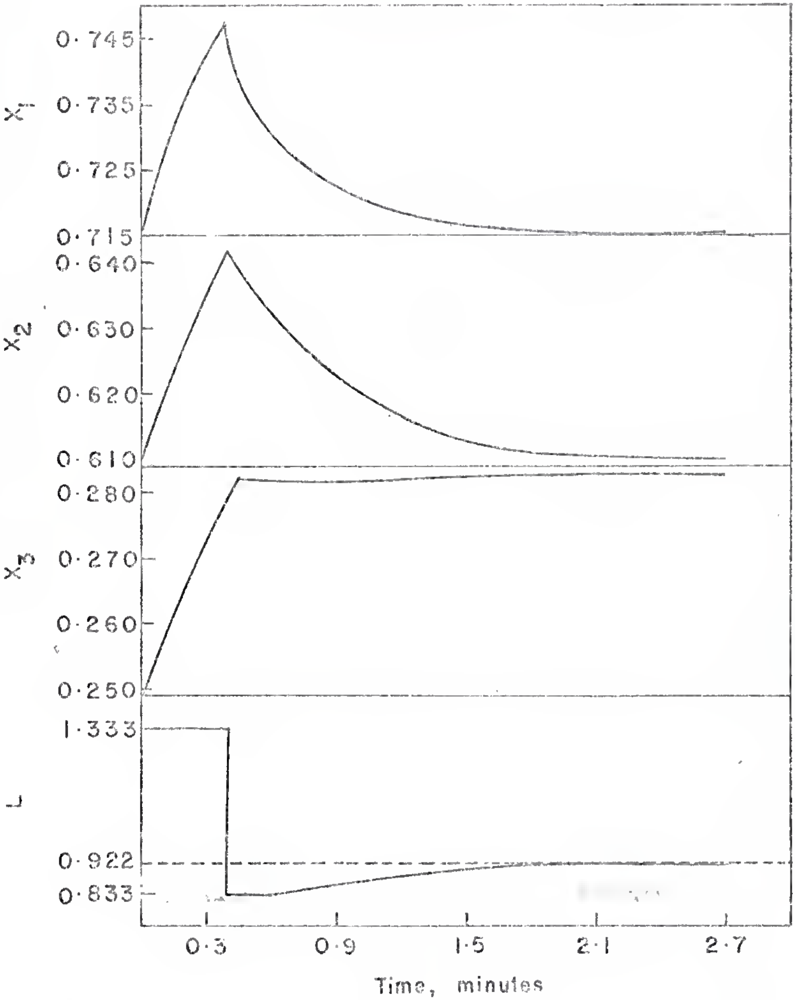


Fig.34. Response of the two tanks in series system to singular control (Case.4.) for time optimal problem.

The second type (in Case 4) uses L_{max} initially until the first switch after which L_{min} is used until a second switch after which singular control is used. In all four cases the control variable L tends to a final value of L_1' and as a result the system approaches the desired final state saymptotically without overshoot (in contrast to the case of the reference system where purely bang bang control was used) and maintains the desired final state. The results for the four cases are tabulated in Table 2. In Figure 35 a comparison is made between the bang-bang policy as obtained from the reference system analysis and the singular policy as obtained from the mixing pool model system analysis, for the time optimal problem.

The method of Grethlein and Lapidus [15] was also applied to the time optimal problem for the Reference system treated in Chapter 2. The original objective function in equation (12), i.e. $\int_0^T dt$, was replaced by a weighted least squares objective function and the procedure described above was carried out to obtain a time optimal policy. These results are compared, in Table 3, with the rigorously determined bang-bang policy of Chapter 2, and the corresponding responses are compared in Figures 36, 37, 38 and 39. It is quite evident that the bang-bang policy does indeed achieve time optimality. The responses from the two policies differ only in that the singular response approaches the final desired state asymptotically, while the bang-bang response tends to overshoot at the final state.

TABLE 2

RESULTS OF THE TIME OPTIMAL PROBLEM FOR THE TWO TANKS-IN-SERIES SYSTEM (OBJECTIVE FUNCTION USED IS THE WEIGHTED LEAST SQUARES TYPE IN EQUATION (54)).

	Weighting factors used in equation (54)	Order in which control is applied	Switching times t_s, min.	Final time T, min
Case 1	a = b = 0.01 C = 1	Start with L_{max} end with singular control	1.45	3.45
Case 2	a = b = 0.001 C = 1	Start with L_{max} end with singular control	2.30	4.15
Case 3	a = b = 0.0001 C = 1	Start with L_{max} end with singular control	5.90	7.35
Case 4	a = b = 0.01 C = 1	Start with L_{max} switch to L_{min} and end with singular control	0.40 0.60	2.71

TABLE 3

COMPARISON OF RESULTS FROM BANG-BANG (OBJECTIVE FUNCTION IS $\int_0^T dt$) AND SINGULAR (OBJECTIVE FUNCTION IS OF THE WEIGHTED LEAST SQUARES TYPE) POLICIES OF THE TIME OPTIMAL PROBLEM FOR THE REFERENCE SYSTEM.

	Bang Bang	Singular
	Final time T, min	Final time T, min
Case 1	2.8	4.85
Case 2	4.05	5.45
Case 3	8.16	8.46
Case 4	1.68	4.3

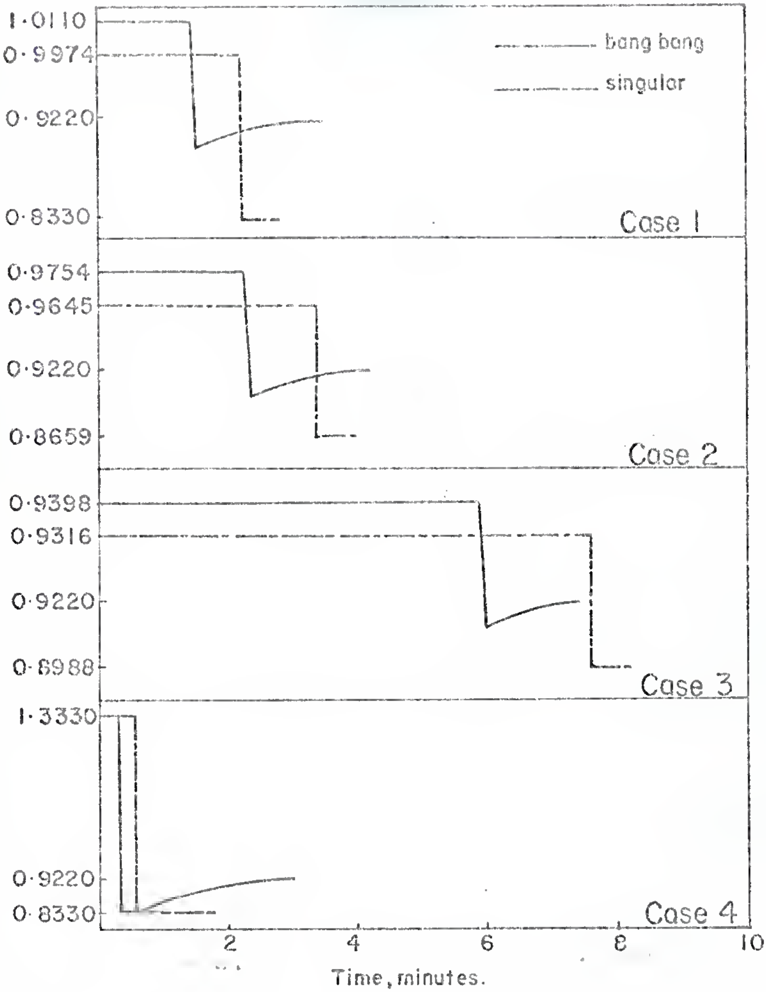


Fig. 35. Comparison of bang bang (reference system) and singular (two tanks in series system) control policies for the time optimal problem.

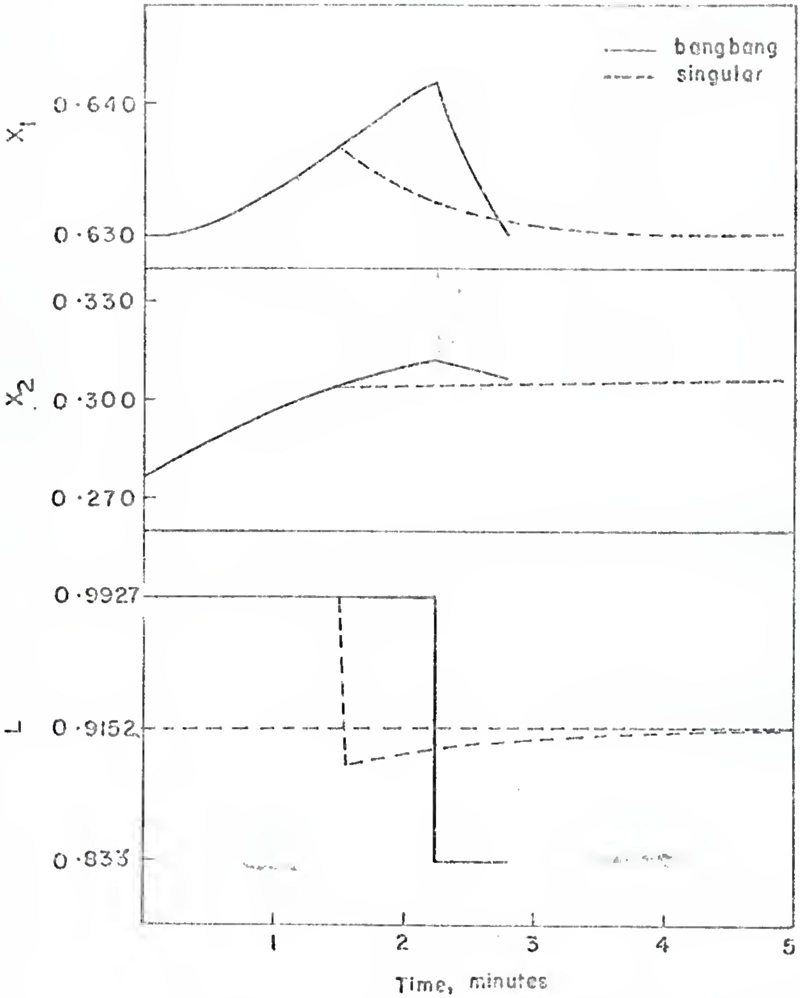


Fig.36. Comparision of reference system responses to bang-bang and singular policies for the time optimal problem (case.I.).

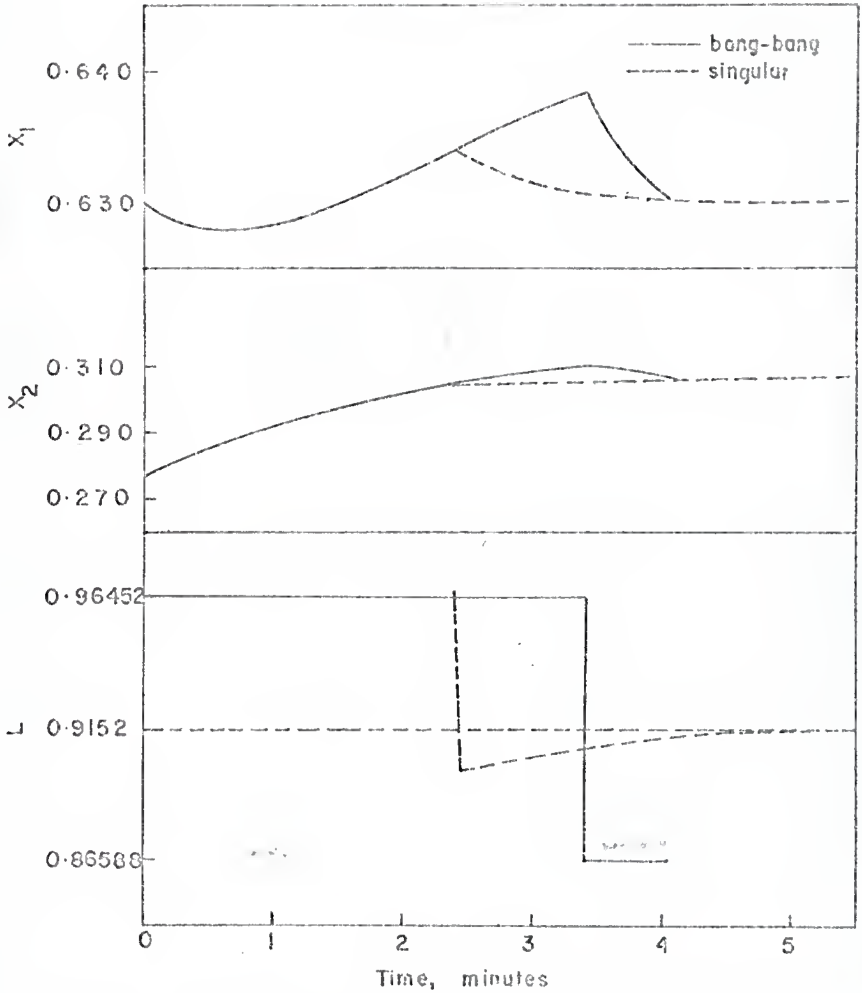


Fig.37. Comparison of reference system responses to bang bang and singular policies for the time optimal problem (Case 2).

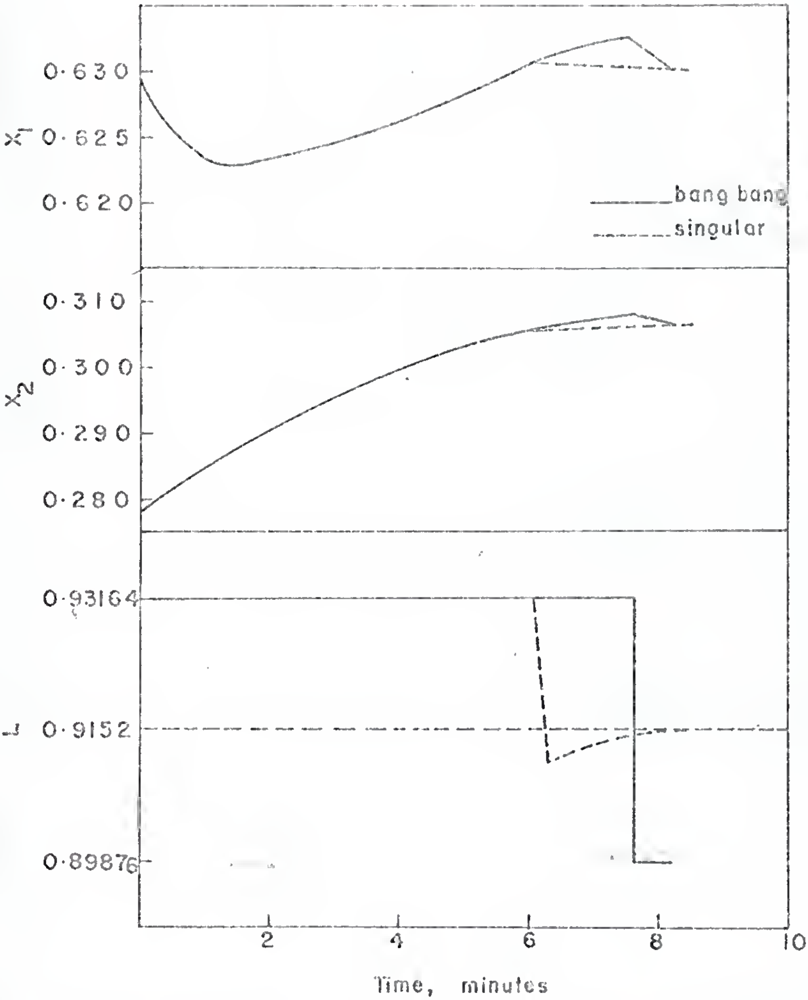


Fig.38. Comparison of reference system responses to bang bang and singular policies for the time optimal problem (Case 3).

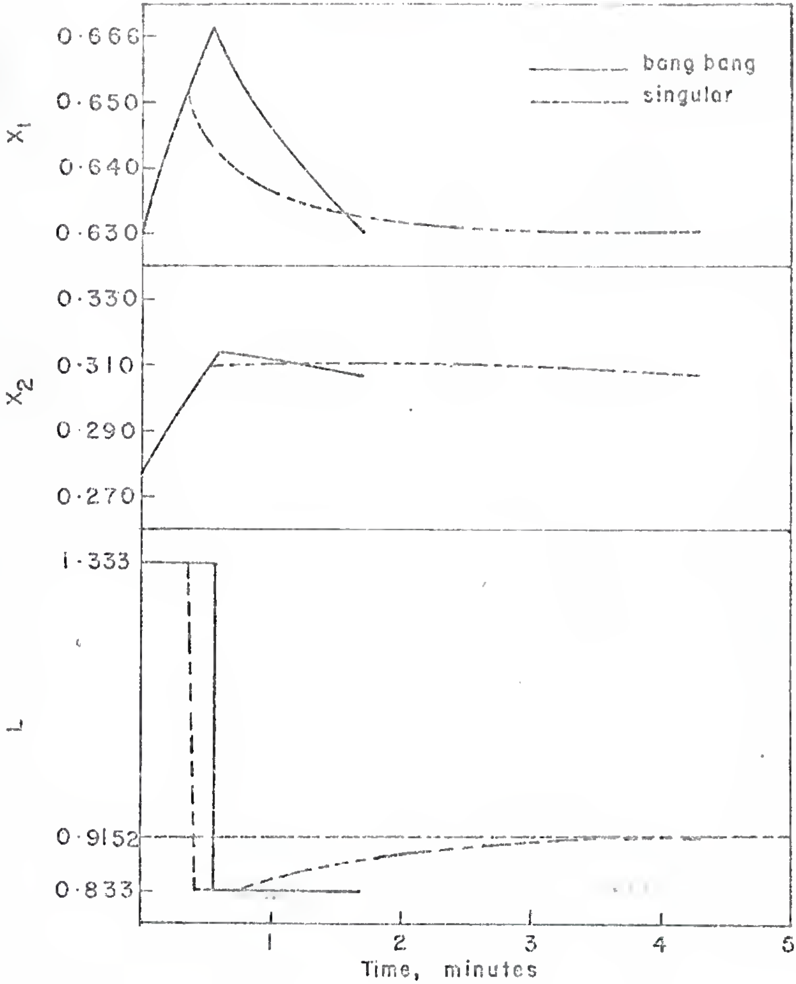


Fig.39. Comparison of reference system responses to bang bang and singular policies for the time optimal problem. (case 4).

CHAPTER 4

CONTROL WHICH IS OPTIMUM IN THE SENSE OF MINIMUM TOTAL DEVIATION

In this chapter attention will be focussed on the minimization of an objective function of the form

$$S = \int_0^T [x^* - x(t)]^2 dt$$

which is a measure of the deviation from some desired quantity x^* over the unspecified time interval T. A control policy L(t) is sought, which transfers the system from some known initial state to a desired final state such that S is minimized.

The two systems which will be subjected to such a minimization are the reference system and the system with the mixing condition on the top tray described by the two-tanks in-series model.

1. REFERENCE SYSTEM

In this section we shall consider the reference system only. The performance equations of the system are those of Chapter 2 and are repeated here for convenience

$$\frac{dx_1}{dt} = \frac{(Lm - Vm - L)}{H_T}x_1 + \frac{Vm}{H_T}x_2 + \frac{Lc}{H_T} \tag{55}$$

$$\frac{dx_2}{dt} = \frac{L}{H_B}x_1 - \frac{(Vm + F + L - V)}{H_B}x_2 + \frac{Fx_F - Vc}{H_B} \tag{56}$$

The boundary conditions are

$x_1(0) = 0.6300 \qquad x_1(T) = 0.6300$

$x_2(0) = 0.2767 \qquad x_2(T) = 0.3067$

where T is unfixed.

The problem is to determine the control L(t) such that the system is transferred from the initial state $S_1 \equiv (0.6300, 0.2767)$ to the final state $S_2 \equiv (0.6300, 0.3067)$ simultaneously minimizing the objective function

$$S = \int_0^T [x_D^* - x_D(t)]^2 \, dt$$

where

$x_D^* = 0.837 \qquad$ [cf. equation (7)]

$x_D(t) = y_1 = 0.44x_1(t) + 0.56 \qquad$ [cf. equatien (7)]

and the final time T is unspecified. Thus we essentially want to minimize

$$S = \int_0^T [0.837 - 0.44x_1(t) - 0.56]^2 \, dt \tag{57}$$

Introducing an additional state variable, we have

$$x_3(T) = S' = \int_0^T [0.837 - 0.44x_1(t) - 0.56]^2 dt$$

or

$$\frac{dx_3}{dt} = [0.837 - 0.44x_1 - 0.56]^2; \quad x_3(0) = 0 \tag{58}$$

The Hamiltonian for the system becomes

$$H = \left(\frac{Lm - Vm - L}{H_T}\right)x_1 z_1 + \frac{Vm}{H_T}x_2 z_1 + \frac{Lc}{H_T}z_1 + \frac{L}{H_B}x_1 z_2$$

$$- \left(\frac{Vm + F + L - V}{H_B}\right)x_2 z_2 + \frac{(Fx_F - Vc)}{H_B} z_2$$

$$+ [0.837 - mx_1 - c]^2 z_3 \qquad (59)$$

The adjoint equations can be derived from the Hamiltonian

$$\frac{dz_1}{dt} = - \left(\frac{Lm - Vm - L}{H_T}\right)z_1 - \frac{L}{H_B}z_2 + 2m(0.837 - mx_1 - c)z_3$$

$$(60)$$

$$\frac{dz_2}{dt} = - \frac{Vm}{H_T} z_1 + \left(\frac{Vm + F + L - V}{H_B}\right) z_2 \qquad (61)$$

$$\frac{dz_3}{dt} = 0 \qquad (62)$$

The boundary conditions on the adjoint variables are

$z_1(0)$ unspecified $\qquad$ $z_1(T)$ unspecified

$z_2(0)$ unspecified $\qquad$ $z_2(T)$ unspecified

$z_3(0)$ unspecified $\qquad$ $z_3(T) = 0$

Equation (62) along with the boundary condition on z_3 implies that

$$z_3 = 1, \qquad 0 \le t \le T$$

Making use of the property that the minimum of the Hamiltonian is zero when T is unspecified, we have

$$H = \left(\frac{mz_1x_1}{H_T} - \frac{x_1z_1}{H_T} + \frac{cz_1}{H_T} + \frac{x_1z_2}{H_B} - \frac{x_2z_2}{H_B}\right)L + \frac{Vm\ x_2z_1}{H_T} - \frac{Vm\ x_1z_1}{H_T}$$

$$- \frac{Vm\ x_2z_2}{H_B} - \frac{(F - V)x_2z_2}{H_B} + \frac{(Fx_F - Vc)z_2}{H_B}$$

$$+ [0.837 - mx_1 - c]^2 = 0 \qquad (63)$$

wherein the Hamiltonian has been rearranged and shown linear in the control variable L. Once more a bang-bang policy is indicated whereby

$$L = L_{max} \text{ if } \left(\frac{mz_1x_1}{H_T} - \frac{x_1z_1}{H_T} + \frac{cz_1}{H_T} + \frac{x_1z_2}{H_B} - \frac{x_2z_2}{H_B}\right) < 0 \qquad (64)$$

or

$$L = L_{min} \text{ if } \left(\frac{mz_1x_1}{H_T} - \frac{x_1z_1}{H_T} + \frac{cz_1}{H_T} + \frac{x_1z_2}{H_B} - \frac{x_2z_2}{H_B}\right) > 0$$

Comparing equations (63) and (64) with equations (21) and (21a) respectively it appears that the minimum total deviation and time optimal problems have similar solutions. As a matter of fact, the performance equations being the same for the two cases, the phase planes are identicaland hence the bang-bang policy obtained for the time optimal problem seems to be feasible for the minimum total deviation problem. However, this is not so. The trial and error method outlined in Figure 5 was applied to the present problem wherein the initial value of z_2 was assumed and the initial value of z_1 was obtained from

$$z_1(0) = - \frac{0.1413\ L(0) - 0.1213}{0.2071\ L(0) - 0.2071}\ z_2(0) \qquad (65)$$

Equation (65) is the analog of equation (22) in the time optimal case. A bang-bang policy was obtained for the four cases investigated in Chapter 2 i.e.

Case 1	$L_{min} = 0.833$	$L_{max} = 0.9974$
Case 2	$L_{min} = 0.86588$	$L_{max} = 0.96452$
Case 3	$L_{min} = 0.89876$	$L_{max} = 0.93164$
Case 4	$L_{min} = 0.833$	$L_{max} = 1.333$

however, the Hamiltonian retained a positive value along the optimal response, instead of attaining a minimum at zero for all four cases, thus indicating that the objective function could not be minimized by mere bang-bang control. Once more a singular policy was obtained by using the method of Grethlein and Lapidus [15].

In order to apply the singular control method a modified objective function was defined of the form

$$J(N) = \sum_{k=1}^{N} S(k) \qquad N \rightarrow \infty \tag{66}$$

with

$$S(k) = [0.837 - 0.44\, x_1 - 0.56]^2 \tag{67}$$

Equation (67) should be interpreted as

$$S(k) = [x_D^* - x_D(t)]^2$$

where

$$x_D^* = 0.837$$

and

$$x_D(t) = 0.44\, x_1 - 0.56 \qquad \text{[cf. equation (7)]}$$

Note that in equation (67) the weighting factor is taken as unity. The sequence of control variables was selected so as to minimize equation (67) at each sampling point in time. Also, the variable $x_3(t)$ as defined by equation (58) was evaluated all along the optimal trajectory (optimal with respect to equation (66)). Recall that $x_3(T)$ (T is the time at which the final desired state is reached) is indeed the objective function that we originally wished to minimize according to equation (58). It was found that $x_3(T)$ as obtained by the singular policy is indeed lower then $x_3(T)$ as obtained by the bang-bang policy. Comparison of the two is made in Table 4, for all four cases. The response to the singular policy is shown in Figures 40, 41, 42 and 43. The response to the bang-bang policy is identical to that in Figures 15, 16, 17 and 18. In Figure 44, comparison is made of the control policies resulting from bang-bang and singular control. Rather significant differences can be seen in the form of control as well as the duration of control. Though acheiving a smaller deviation, singular control must be applied for a longer time while bang-bang control which does not acheive as small a deviation as singular control is applied for a very short time. It seems as though in a practical situation the most likely objective function to minimize would

TABLE 4

COMPARISON OF RESULTS FROM BANG-BANG AND SINGULAR POLICIES FOR MINIMUM DEVIATION PROBLEM (REFERENCE SYSTEM)

	Bang-Bang		Singular	
	Total minimum deviation $x_3(T)$	Final time T, min.	Total minimum deviation $x_3(T)$	Final time T, min
Case 1	0.2154×10^{-4}	2.80	0.3800×10^{-6}	7.70
Case 2	0.1034×10^{-4}	4.05	0.6730×10^{-6}	7.80
Case 3	0.2583×10^{-4}	8.16	0.24871×10^{-4}	9.90
Case 4	0.1031×10^{-3}	1.68	0.3680×10^{-6}	7.60

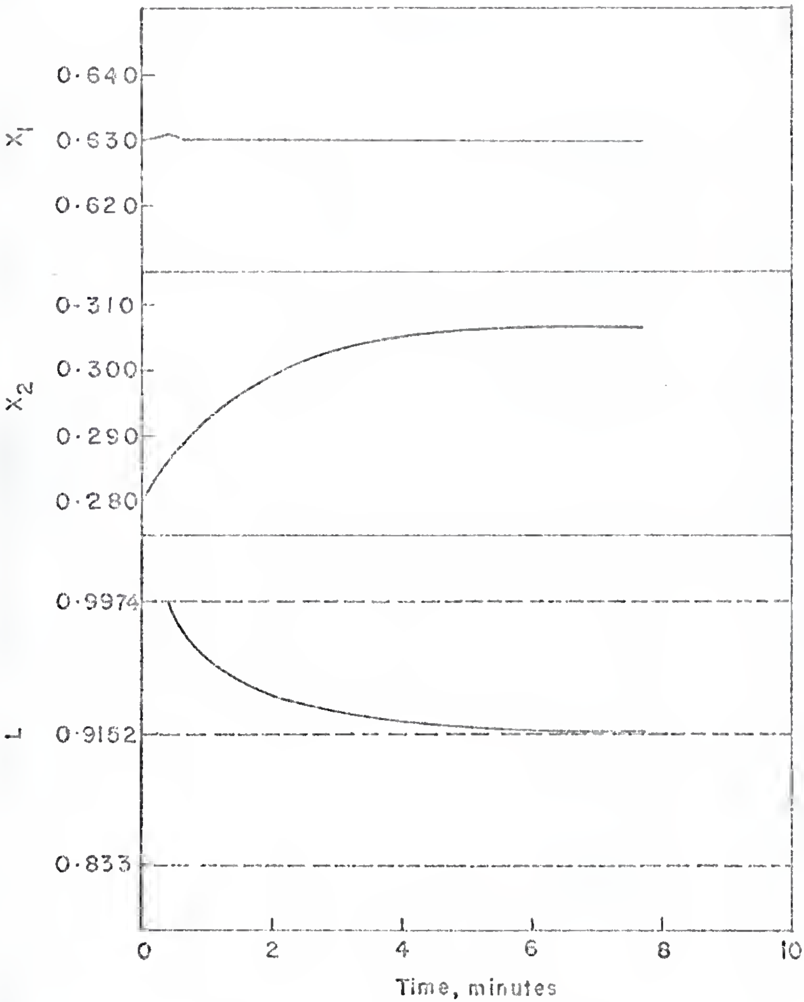


Fig. 40. Response of reference system to the singular policy for the minimum deviation problem (Case I).

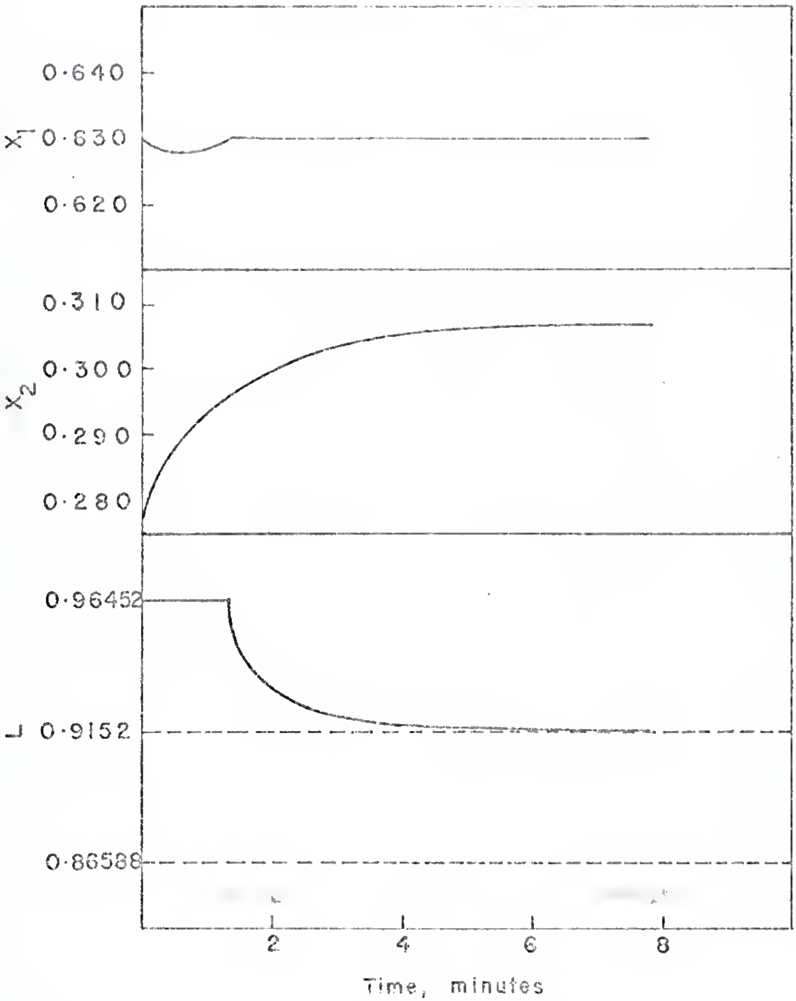


Fig.41. Response of reference system to the singular policy for the minimum deviation problem(Case2).

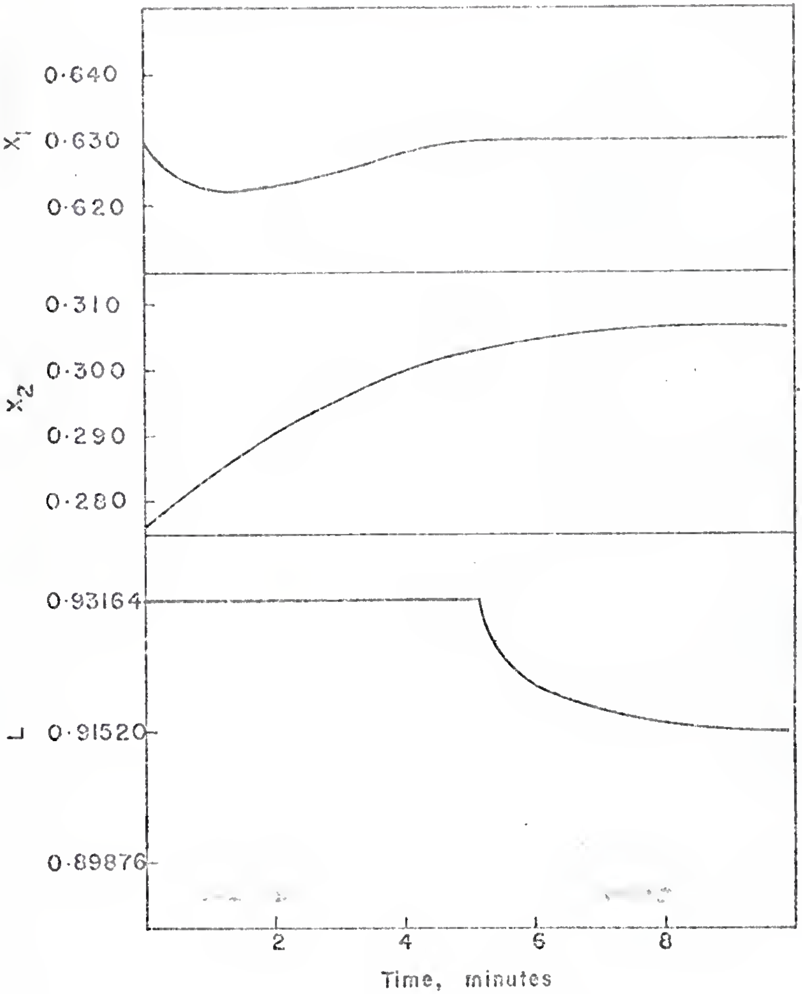


Fig.42. Response of reference system to the singular policy for the minimum deviation problem(Case 3).

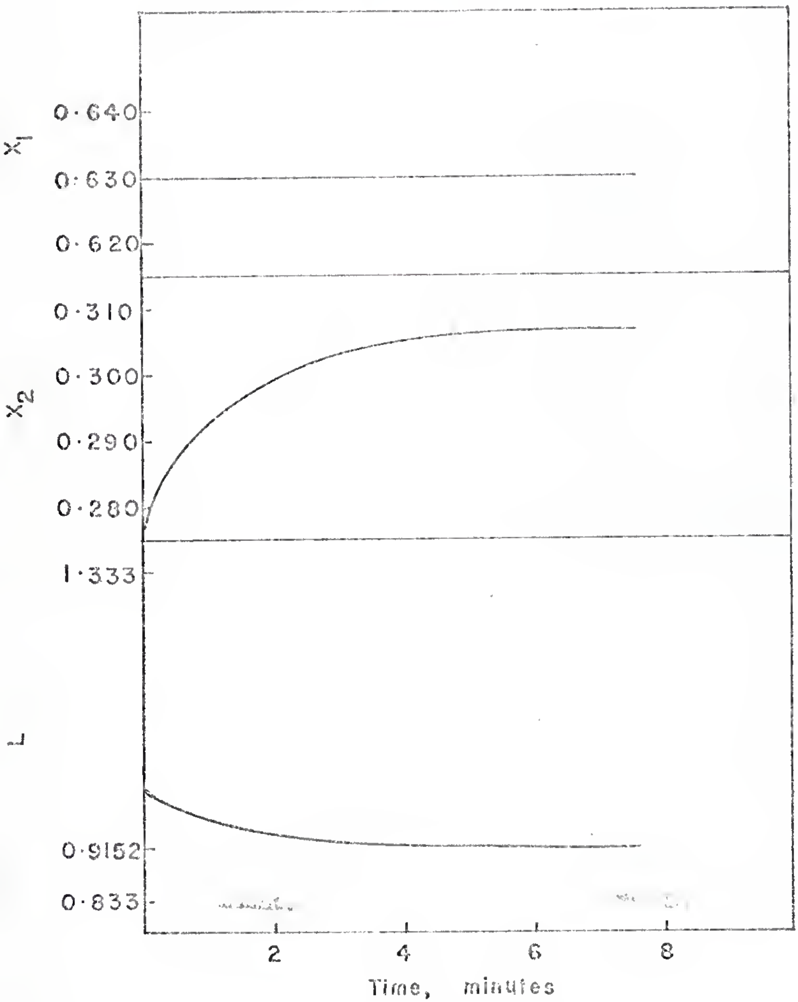


Fig. 43. Response of reference system to the singular policy for the minimum deviation problem (Case 4).

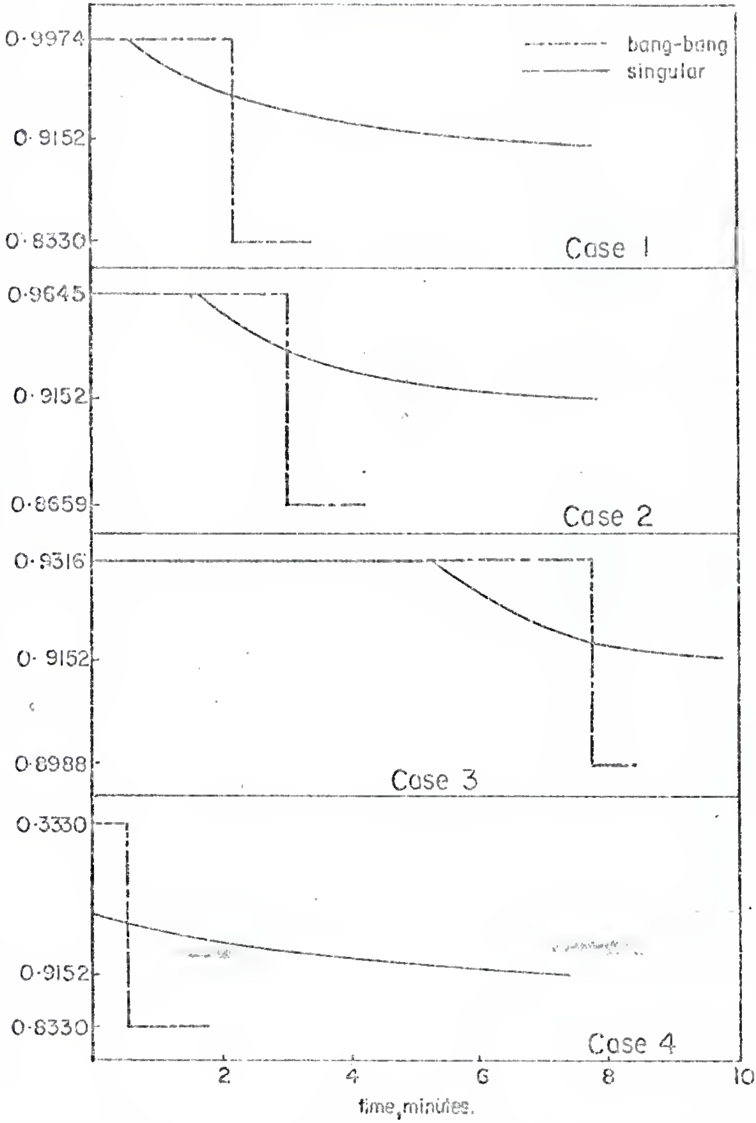


Fig.44. Comparison of bang bang and singular control policies as applied to the minimum deviation problem and the reference system.

be of the type

$$S = \int_0^T \left\{ [x_D^* - x_D(t)]^2 + 1 \right\} dt$$

wherein a compromise is made between minimum time and minimum deviation.

2. SYSTEM WITH TOP TRAY DESCRIBED AS TWO TANKS IN SERIES

The performance equations of Chapter 3 are repeated here for convenience.

$$\frac{dx_1}{dt} = (\frac{Lm - Vm - 2L}{H_T})x_1 + \frac{Lm}{H_T}x_2 + \frac{Vm}{H_T}x_3 + \frac{2Lc}{H_T} \tag{68}$$

$$\frac{dx_2}{dt} = \frac{2L}{H_T} x_1 - (\frac{2L + Vm}{H_T})x_2 + \frac{Vm}{H_T} x_3 \tag{69}$$

$$\frac{dx_3}{dt} = \frac{L}{H_B}x_2 - (\frac{Vm + F + L - V}{H_B})x_3 + \frac{Fx_F - Vc}{H_B} \tag{70}$$

and the boundary conditions are

$x_1(0) = 0.71467$ $\qquad$ $x_1(T) = 0.71399$

$x_2(0) = 0.60909$ $\qquad$ $x_2(T) = 0.60986$

$x_3(0) = 0.24899$ $\qquad$ $x_3(T) = 0.28247$

where T is unfixed.

The problem, once again, is to determine the control L(t) which will transfer the system from the initial state $S'_1 \equiv (0.71467, 0.60909, 0.24899)$ to the final state $S'_2 \equiv (0.71399, 0.60986, 0.28247)$ and in so doing will minimize the objective function

$$S = \int_0^T [x_D^* - x_D(t)]^2 dt$$

where

$$x_D^* = 0.85123 \qquad [\text{cf. equation (27)}]$$

$$x_D(t) = 0.22x_1 + 0.22x_2 + 0.56 \qquad [\text{cf. equation (27)}]$$

and the final time T is unfixed. Thus, essentially we have to minimize

$$S' = \int_0^T [0.85123 - 0.22x_1 - 0.22x_2 - 0.56]^2 \, dt \tag{71}$$

Next a new variable x_4 is introduced such that

$$x_4(T) = S' = \int_0^T [0.85123 - 0.22x_1 - 0.22x_2 - 0.56]^2 dt$$

or

$$\frac{dx_4}{dt} = [0.85123 - 0.22x_1 - 0.22x_2 - 0.56]^2; \quad x_4(0) = 0 \tag{72}$$

The Hamiltonian for the system becomes

$$\begin{aligned} H = {} & \left(\frac{Lm - Vm - 2L}{H_T}\right)x_1z_1 + \frac{Lm}{H_T}x_2z_1 + \frac{Vm}{H_T}x_3z_1 + \frac{2Lc}{H_T}z_1 \\ & + \frac{2L}{H_T}x_1z_2 - \left(\frac{2L + Vm}{H_T}\right)x_2z_2 + \frac{Vm}{H_T}x_3z_2 + \frac{L}{H_B}x_2z_3 \\ & - \left(\frac{Vm + F + L - V}{H_B}\right)x_3z_3 + \left(\frac{Fx_F - Vc}{H_B}\right) z_3 \\ & + [0.85123 - 0.22x_1 - 0.22x_2 - 0.56]^2 z_4 \end{aligned} \tag{73}$$

and the adjoint differential system derived from the Hamiltonian is,

$$\frac{dz_1}{dt} = -\left(\frac{Lm - Vm - 2L}{H_T}\right)z_1 - \frac{2L}{H_T}z_2$$

$$+ 0.44[0.85123 - 0.22x_1 - 0.22x_2 - 0.56]z_4 \qquad (74)$$

$$\frac{dz_2}{dt} = -\frac{Lm}{H_T}z_1 + \left(\frac{2L + Vm}{H_T}\right)z_2 - \frac{L}{H_B}z_3$$

$$+ 0.44[0.85123 - 0.22x_1 - 0.22x_2 - 0.56]z_4 \qquad (75)$$

$$\frac{dz_3}{dt} = -\frac{Vm}{H_T}z_1 - \frac{Vm}{H_T}z_2 + \left(\frac{Vm + F + L - V}{H_B}\right)z_3 \qquad (76)$$

$$\frac{dz_4}{dt} = 0 \qquad (77)$$

and the boundary conditions on the adjoint variables are

$$\begin{array}{ll} z_1(0) \text{ unspecified} & z_1(T) \text{ unspecified} \\ z_2(0) \text{ unspecified} & z_2(T) \text{ unspecified} \\ z_3(0) \text{ unspecified} & z_3(T) \text{ unspecified} \\ z_4(0) \text{ unspecified} & z_4(T) = 1. \end{array} \qquad (78)$$

From the final condition on z_4 and equation (74), it follows that

$$z_4 = 1, \qquad 0 \leq t \leq T$$

The Hamiltonian can be rewritten as follows,

$$H = (mx_1z_1 - 2x_1z_1 + mx_2z_1 + 2cz_1 + 2x_1z_2 - 2x_2z_2$$

$$+ \frac{x_2 z_3}{H_B} - \frac{x_3 z_3}{H_B})L + Vmx_3 z_1 - Vmx_1 z_1 - Vmx_2 z_2 + Vmx_3 z_2$$

$$- \frac{Vmx_3 z_3}{H_B} - \frac{(F - V)}{H_B} x_3 z_3 + (\frac{Fx_F - Vc}{H_B}) z_3$$

$$+ [0.85123 - 0.22x_1 - 0.22x_2 - 0.56]^2 \qquad (79)$$

wherein the H_T has been omitted since it has a value of unity. Also the Hamiltonian is shown linear in the control variable L, thus implying a bang-bang policy. The switching function of the bang-bang policy is identical with equation (44) which is not unexpected. From the analysis of phase planes in Chapter 3 it was shown that the final state could not be reached by purely bang-bang control and hence in the present problem we straightaway resort to singular control.

In order to apply the singular control method a modified objective function was defined of the form

$$J(N) = \sum_{k=1}^{N} S(k) \qquad N \rightarrow \infty \qquad (80)$$

with

$$S(k) = [0.85123 - 0.22x_1 - 0.22x_2 - 0.56]^2 \qquad (81)$$

Equation (81) should be interpreted as

$$S(k) = [x_D^* - x_D(t)]^2$$

where

$$x_D^* = 0.85123$$

and

$$x_D(t) = 0.22x_1 + 0.22x_2 + 0.56 \qquad \text{[cf. equation (72)]}$$

Note that in equation (81) the weighting factor has been taken as unity. The sequence of control variables was determined so as to minimize equation (81) at each sampling point in time. Also, the variable $x_4(t)$ as defined by equation (72) was evaluated all along the optimal trajectory (optimal with respect to equation (80)). The following four cases were investigated

Case 1. $L_{min} = 0.833$ $\quad L_{max} = 1.011$

Case 2. $L_{min} = 0.8686$ $\quad L_{max} = 0.9754$

Case 3. $L_{min} = 0.9042$ $\quad L_{max} = 0.9398$

Case 4. $L_{min} = 0.833$ $\quad L_{max} = 1.333$

and the corresponding values of $x_4(T)$ are presented in Table 5. The response of the system for the four cases is plotted in Figures 45, 46, 47 and 48.

TABLE 5

RESULTS OF MINIMUM DEVIATION PROBLEM FOR SYSTEM WITH TOP TRAY DESCRIBED AS TWO TANKS IN SERIES

	Final time T, min.	Minimum deviation $x_4(T)$
Case 1	9.50	0.1×10^{-8}
Case 2	9.60	0.227×10^{-6}
Case 3	10.95	0.25×10^{-4}
Case 4	9.40	0.1×10^{-9}

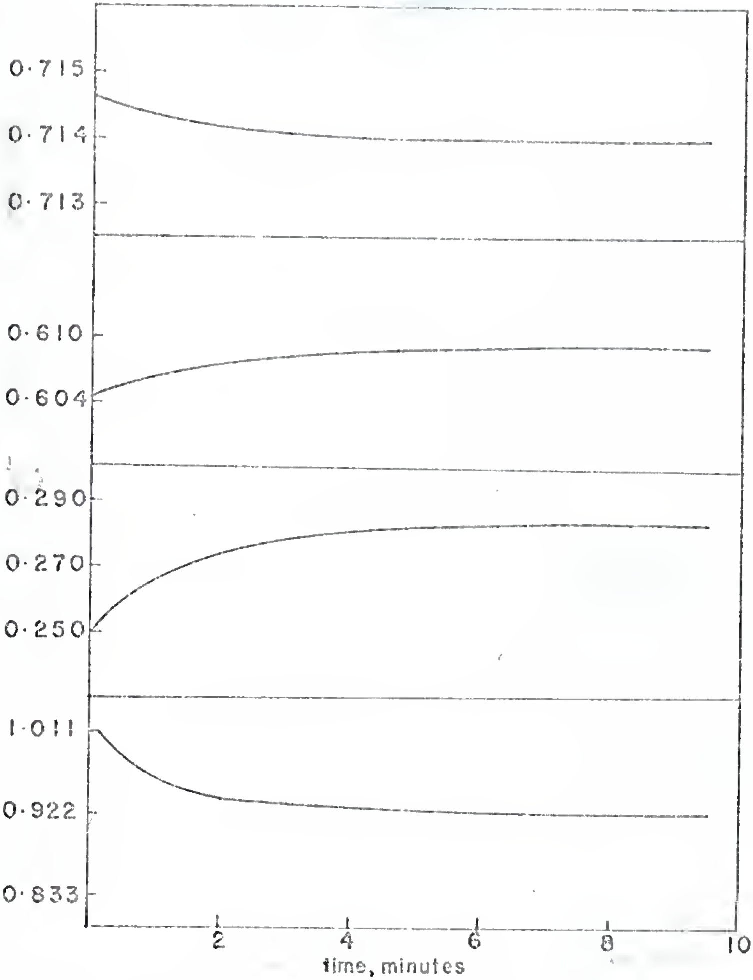


Fig.45. Response of the two tanks in series system to singular control for the minimum deviation problem (Case. I.)

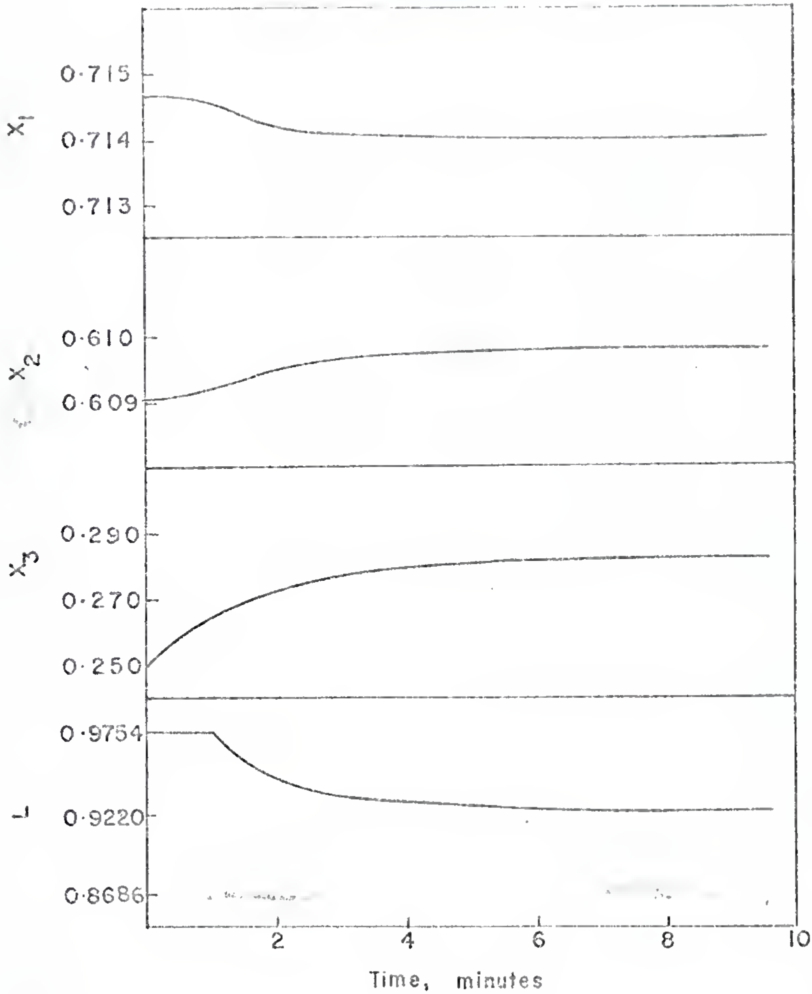


Fig.46. Response of the two tanks in series system to singular control for the minimum deviation problem (Case 2).

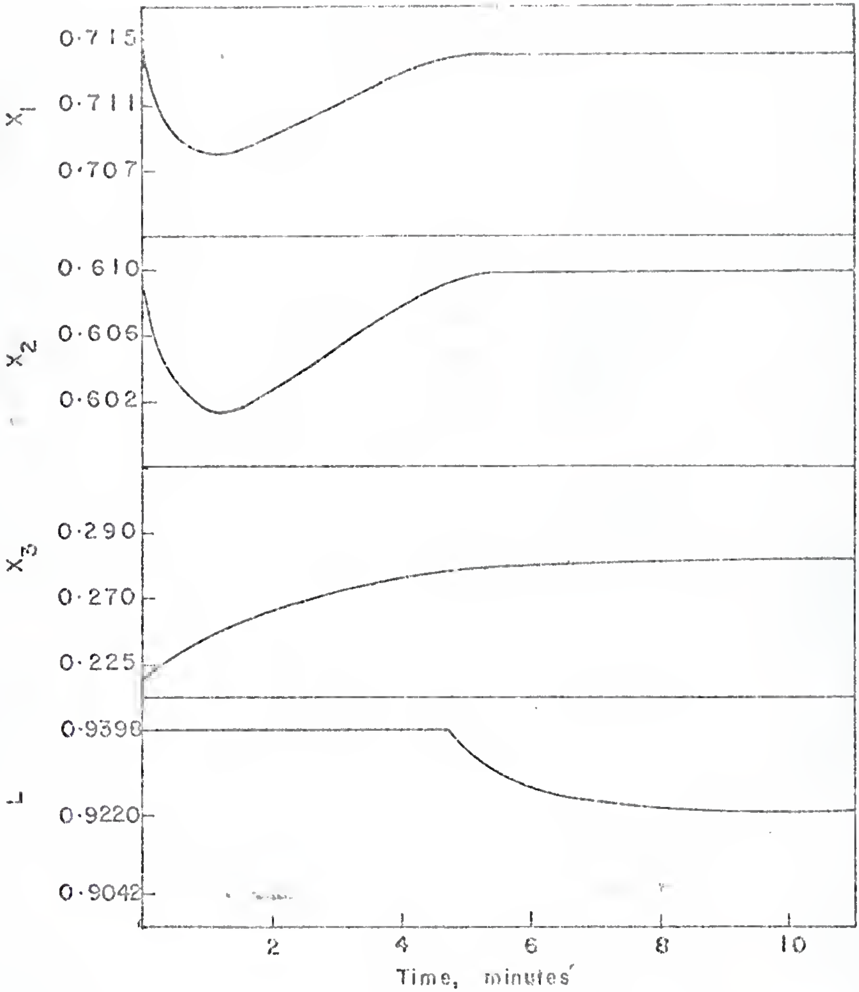


Fig. 47. Response of the two tanks in series system to singular control for the minimum deviation problem (Case 3.).

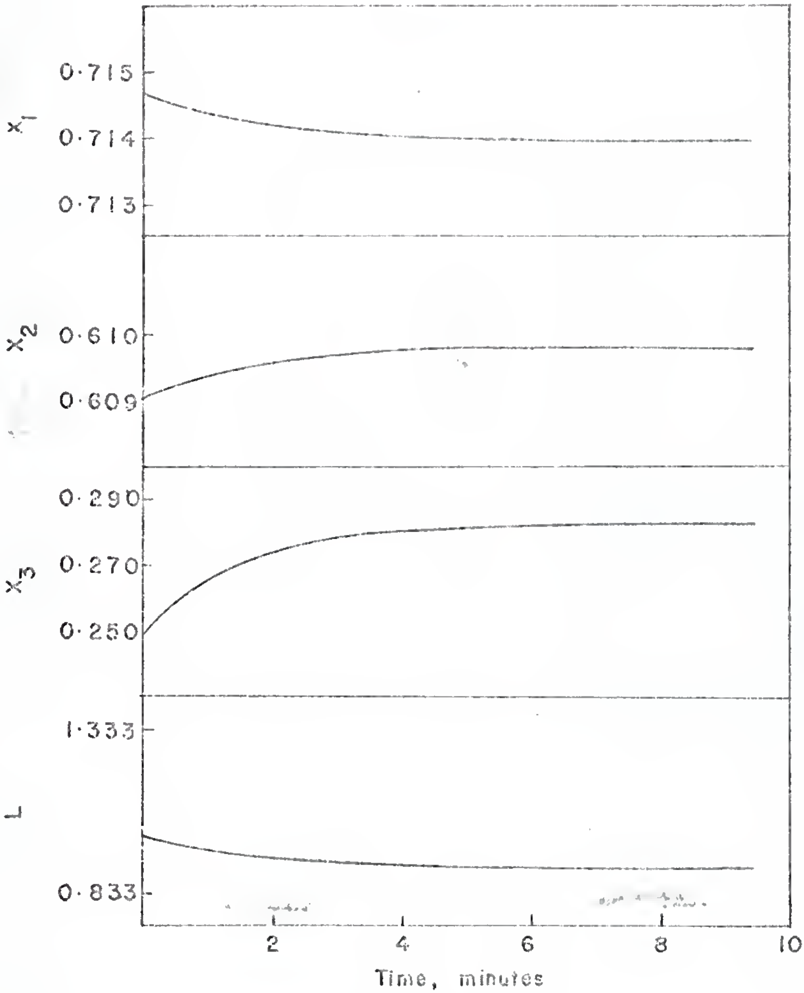


Fig. 48. Response of the two tanks in series system to singular control for the minimum total deviation problem.(case 4.)

CHAPTER 5

SUMMARY OF RESULTS, CONCLUSIONS AND RECOMMENDATIONS

The results presented in the preceeding chapters demonstrate the variations in control policy and also in the methods for obtaining the same when the tanks-in-series model is substituted for the conventional completely mixed tray. The mathematical models used were adequate to represent the phenomenon to be investigated without having to go into the complexities of the hydrodynamics or the energy balance of the system. Basically two types of problems have been treated, the time optimal problem, and the minimum deviation problem.

In Chapter 2, the reference system (conventional completely mixed single tank model) was set up and the time optimal problem was treated. The control policy was determined so as to transfer the system from some initial state to a desired final state in the shortest possible time. The optimal control as determined via the Maximum Principle was found to be purely bang-bang and the results are presented in Table 1 and Figures 15, 16, 17 and 18.

In Chapter 3, the two tanks in series system was set up and the time optimal problem was once again treated. Herein was noticed the first change in control policy. It was found that the final desired state could not be attained by merely using bang-bang control and hence singular control was resorted to. The results are presented in Table 2 and Figure 31, 32, 33, and 34. Also as a check on the barg-bang policy obtained in Chapter 2 with regard to the reference system, the time optimal problem of Chapter 2 was solved again by using singular control. The comparison of results from the two modes of control is made in Table 3 and Figures 36, 37, 38 and 39, from which it was quite evident that for the reference system, the bang-bang policy indeed achieves time optimality.

Next the minimum deviation problem was considered in Chapter 4 for both systems. For the reference system it seemed quite obvious that bang-bang control should suffice once more, as it did for the time optimal problem, however, the results turned out quite opposite to the obvious, and in truth singular control had to be used to obtain minimum deviation optimality. This was confirmed by comparison with the bang-bang response in Table 4.

Perhaps it should be pointed out at this stage that a significant observation made from the results of this thesis is the different conditions under which the necessity for singular control should be recognized. The usual conditions is that the switching function becomes zero over a positive interval of time, however, as pointed out by Johnson [12], it is not always possible to detect this when ordinary computer searching methods are used. Another condition is that sometimes the desired final conditions on the state variables cannot be attained by merely using bang-bang control. When such a situation occurs it is only natural that singular control be used to achieve the final state and hence perhaps optimality. This was the situation encountered in Chapter 3 with the two tanks in series system and the time optimal problem. In the case where the final state can be arrived at by bang-bang control, a check has to be made on the Hamiltonian to see whether it has stayed at its minimum throughout the transient response (in the case where the final time is unspecified, this minimum is zero). If the Hamiltonian maintains a non zero value then this is an indication that even though the bang-bang policy gets us to where we want to go, in doing so it does not achieve the desired optimality and thus singular control has to be used. This precisely is what happened in Chapter 4 when the minimum deviation problem was being considered with the reference system. Also the superiority of the singular policy over the bang-bang policy in achieving a minimum deviation is shown in Table 4.

In the latter part of Chapter 4, the minimum deviation problem is applied to the mixing pool system and results are tabulated in Table 5 and corresponding responses are shown in Figures 45, 46, 47 and 48. A singular policy was used to achieve a minimum deviation.

In Tables 6 and 7 are given the comparisons of response times of the reference system and the two tanks in series system, for the time optimal and minimum deviation problems respectively. Only responses from singular control policies are considered. From Table 6 we see that for the time optimal problem the reference system has a slower optimal response time than the two tanks in series system while from Table 7 we see that for the minimum deviation problem the reference system has a faster

TABLE 6

COMPARISON OF RESPONSE TIMES TO SINGULAR CONTROL POLICIES AS APPLIED TO THE REFERENCE SYSTEM AND THE TWO TANKS IN SERIES SYSTEM (TIME OPTIMAL PROBLEM)

	Reference System T, min	Two tanks in series system T, min
Case 1	4.85	3.45
Case 2	5.45	4.15
Case 3	8.46	7.35
Case 4	4.30	2.71

TABLE 7

COMPARISON OF RESPONSE TIME TO SINGULAR CONTROL POLICIES AS APPLIED TO THE REFERENCE SYSTEM AND THE TWO TANKS IN SERIES SYSTEM (MINIMUM DEVIATION PROBLEM).

	Reference System T, min	Two tanks in series system T, min
Case 1	7.70	9.50
Case 2	7.80	9.60
Case 3	9.90	10.95
Case 4	7.60	9.40

optimal response time than the two tanks in series system. These results from Tables 6 and 7 show how the response times of a particular system can be quickened or slowed down due to a change in the objcetive function, i.e., dependence of response time on variation in objective function. Similarly other dependences may be noted. For instance in the time optimal problem, in going from the reference system to the two tanks in series system, the control policy changed from bang-bang to singular thus indicating the dependence of control policy on variation in model. Also in the reference system, when going from the time optimal problem to the minimum deviation problem, the control policy changes from bang-bang to singular which shows the dependence of the control policy on changes in objective function when the model is held constant. The problem of meaningfully evaluating these dependences would immediately give rise to a host of sensitivity problems. It may seem vague at this stage to try to obtain expressions for the above sensitivities by the generally accepted perturbation techniques that have been used so far in the automatic control literature. However, as Sridhar et al. [14] have put it, "Sensitivity is a concept which can be meaningfully defined only by considering specific systems and their particular purposes for existence". We do not wish to go into this problem presently but rather point out the possibilities for further research in this area.

To some readers the method of Grethlein and Lapidus [15] may not seem to be a competent method to arrive at a singular policy but, as was stated previously, there is no general method at present by which a singular policy can be decreed optimal. Because of the difficulty in obtaining solutions, the present use of optimization theory for control systems engineering is limited to determining the nature of the optimal control law. This information is useful in evaluating alternate control schemes and in indicating approximations to the optimal control which may be more easily implemented. On a similar note the method of Grethlein and Lapidus was incorporated in the present work not only to achieve simplicity in obtaining a solution but also because of the proven versatility of the method in a somewhat similar problem as described in [15].

The above results, discussion and observations hold only for a particular model with a particular set of parameters, disturbance and initial state. It should be recognized that changes in the various parameters or in the assumptions of Chapters 2 and 3 would lead to diverse situations with diverse results and making any generalizations at this stage may not be prudent.

By way of extensions to the present study several recommendations can be put forth for further study. The question of sensitivity analysis has already been raised in an earlier paragraph. In addition different objective functions could be investigated and especially of the type

$$S = \int_0^T [1 + (x^* - x(t))^2]dt$$

wherein both time and deviation are minimized. Also various modifications can be made on the mixing pool model. In Chapter 3 the assumption was made that the vapor rising from the bottom tray divided into half and each half entered each pool. It would be interesting to study the effect of uneven division of the vapor stream, on the performance of the model. Another problem, of a more complicated nature, is one in which there is feedback between the mixing pools.

As stated above, extensive work has to be done on the present model before any general conclusions can be drawn. However, if the present investigation induces the reader to pursue the subject further, the purpose of this thesis will have been fulfilled.

NOMENCLATURE

B	Bottoms product flow rate, lb mole/min.
c	Constant used in vapor-liquid equilibrium expression, $y = mx + c$.
D	Overheads product flow rate, lb mole/min.
H	Hamiltonian function.
H_B	Bottoms tray, liquid holdup, lb moles.
H_T	Top tray liquid holdup, lb moles.
L	Liquid flow rate in column, lb meles/min.
L'	Reflux flow rate which maintains desired steady state in the two tanks in series system, lb mole/min.
m	Constant used in vapor-liquid equilibrium expression, $y = mx + C$.
S_1, S_2	Initial and terminal states of the reference system.
S_1', S_2'	Initial and terminal states of the two tanks in series system.
T	Terminal time, minutes.
V	Vapor flow rate in column, lb moles/min.
x_1	Light component composition in liquid phase on top tray of reference system. Light component composition in liquid phase in pool 1 of top tray in two tanks in series system.
x_2	Light component composition in liquid phase on bottom tray of reference system. Light component composition in liquid phase in pool 2 of top tray in two tanks in series system.
x_3	Light component composition in liquid phase on bottom tray of two tanks in series system.
y_i	Light component composition in vapor phase in equilibrium with liquid phase of composition x_i.
z_i	Adjoint variable corresponding to state variable x_i.

ACKNOWLEDGEMENTS

The author wishes to express his warmfelt appreciation to his advisor, Prof. L. T. Fan, whose probing questions, careful guidance, and perceptive comments have enriched the contents of this thesis and made its development an enjoyable experience.

The assistance which David Hahn gave in directing the author's efforts along fruitful paths in numerical analysis is gratefully acknowledged. Also continual interest and helpful comments made by Mike Chen are deeply appreciated.

Support for this research extended by the following organizations is greatly appreciated: The National Science Foundation under grant GK-67, The office of Saline Water under grant 14-01-0001-1283.

The computer time made available by the K.S.U. School of Engineering is also worthily appreciated.

REFERENCES

1. Holland, C. D., "Unsteady State Processes with Applications in Multicomponent Distillation", Prentice-Hall, New Jersey (1966).

2. Kirschbaum, E., "Distillation and Rectification", p. 278, Chemical Publishing Co., New York (1948).

3. Gautreaux, H. E., and H. E. O'Connell, Chem. Eng. Progr, 50, 5, 230 (1955).

4. Sakata, M., Chem. Eng. Progr. 62, 11, 98 (1966).

5. Pontryagin, L. S., V. G. Boltyanskii, R. V. Gamkrelidze, E. F. Mischenko, "Mathematical Theory of Optimal Processes", Wiley, New York (1962).

6. Fan, L. T., "The Continuous Maximum Principle", Wiley, New York (1966).

7. Fan, L. T., and C. S. Wang, "The Discrete Maximum Principle", Wiley, New York (1964)

8. Siebenthal, C. D., and R. Aris, Chem. Eng. Sci., 19, 10, 729 (1964).

9. Coward, I., Chem. Eng. Sci., 22, 503 (1967).

10. Coddington, E. A., and N. Levinson, "Theory of Ordinary Differential Equations" McGraw-Hill New York (1955).

11. Javinsky, M. A., and R. H. Kadlec, A.I.Ch.E. Sixty-Third National Meeting, St. Louis, Mo., Feb. (1968).

12. Johnson, C. D. in "Advances in Control Systems", Vol. 2, p. 209, Academic Press, New York, (1965).

13. Markus, L. and Lee, E. B., Arch. Rat. Mech. Anal. 8, 1, 36 (1961).

14. Sridhar, R., R. E. Bellman and R. E. Kalaba, The RAND Corp. RM-4039-PR, Mar. (1964).

15. Grethlein, H. E., and L. Lapidus, A.I.Ch.E.J. Vol. 9, No. 2, p. 230, Mar. 1963.

APPENDIX A

ANALOG AND DIGITAL COMPUTER PROCEDURES

In this section attention will be focussed on the analog computer circuit diagrams and the digital computer programs of the various simulations and computations used in Chapters 2, 3 and 4.

1. ANALOG COMPUTER SIMULATION OF THE REFERENCE SYSTEM.

The system equations used in the simulation of the reference system are those shown in equation (11) namely,

$$\frac{dx_1}{dt} = \left(\frac{Lm - Vm - L}{H_T}\right)x_1 + \frac{Vm}{H_T}x_2 + \frac{Lc}{H_T} \qquad \text{(A-1)}$$

$$-\frac{dx_2}{dt} = -\frac{Lx_1}{H_B} + \left(\frac{Vm + F + L - V}{H_B}\right)x_2 - \frac{Fx_F}{H_B} + \frac{Vc}{H_B}$$

and

$$x_D = mx_1 + c$$

The above equations were magnitude scaled according to the scale factors shown in Table A-1. The corresponding magnitude scaled equations are

$$[\dot{x}_1] = \left(\frac{Lm - Vm - L}{H_T}\right)[x_1] + \frac{Vm}{H_T}[x_2] + \frac{Lc}{H_T}$$

$$-[\dot{x}_2] = -\frac{L}{H_B}[x_1] + \left(\frac{Vm + F + L - V}{H_B}\right)[x_2] - \frac{Fx_F}{H_B} + \frac{Vc}{H_B} \qquad \text{(A-2)}$$

$$[x_D] = m[x_1] + c$$

TABLE A-1

SCALE FACTORS FOR REFERENCE SYSTEM

Problem Variable	Expected Maximum	$\frac{1}{\text{Expected Max.}}$	Scale Factor	Computer Variable
x_1	1.0	1.0	1.0	$[x_1]$
x_2	1.0	1.0	1.0	$[x_2]$
x_D	1.0	1.0	1.0	$[x_D]$

The time scale factor β, defined as the ratio of computer time to the independent problem variable t, was taken as unity; thus one second on the analog computer represents one minute of problem time. The scaled circuit diagram for the reference system is shown in Figure A-1.

2. ANALOG COMPUTER SIMULATION OF THE MIXING POOL MODEL SYSTEM.

The system equations used in the simulation of the mixing pool model system are those shown in equation (32) namely,

$$\frac{dx_1}{dt} = \left(\frac{Lm - Vm - 2L}{H_T}\right) x_1 + \frac{Lm}{H_T} x_2 + \frac{Vm}{H_T} x_3 + \frac{2Lc}{H_T}$$

$$-\frac{dx_2}{dt} = -\frac{2L}{H_T} x_1 + \left(\frac{2L + Vm}{H_T}\right) x_2 - \frac{Vm}{H_T} x_3 \qquad \text{(A-3)}$$

$$\frac{dx_3}{dt} = \frac{L}{H_B} x_2 - \left(\frac{Vm + F + L - V}{H_B}\right) x_3 + \frac{Fx_F - Vc}{H_B}$$

and

$$x_D = 0.5(mx_1 + mx_2 + 2C).$$

The above equations were magnitude scaled according to the scale factors shown in Table A-2. The corresponding magnitude scaled equations are

$$[\dot{x}_1] = \left(\frac{Lm - Vm - 2L}{H_T}\right)[x_1] + \frac{Lm}{H_T}[x_2] + \frac{Vm}{H_T}[x_3] + \frac{2Lc}{H_T}$$

$$-[\dot{x}_2] = -\frac{2L}{H_T}[x_1] + \left(\frac{2L + Vm}{H_T}\right)[x_2] - \frac{Vm}{H_T}[x_3] \qquad \text{(A-4)}$$

$$[\dot{x}_3] = \frac{L}{H_B}[x_2] - \left(\frac{Vm + F + L - V}{H_B}\right)[x_3] + \frac{Fx_F - Vc}{H_B}$$

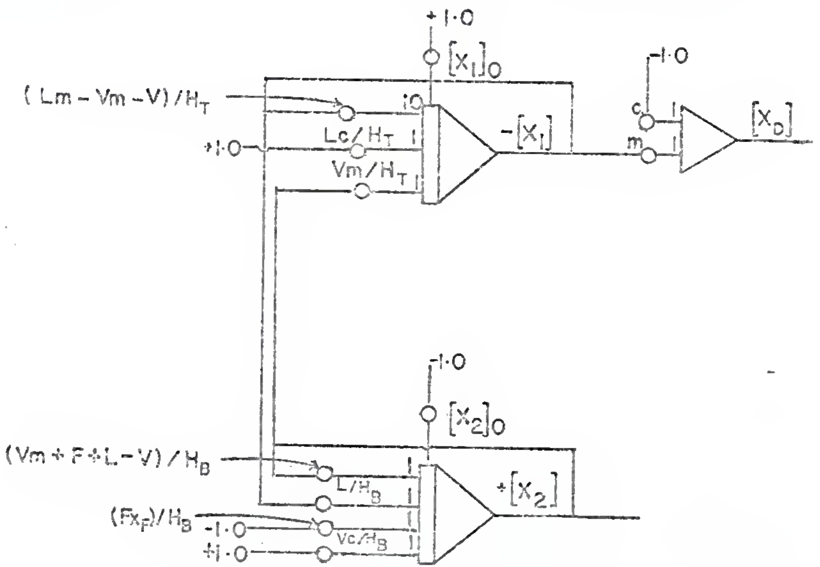


Fig. A-1. Analog computer circuit diagram for equations (A-2).

TABLE A-2

SCALE FACTORS FOR MIXING POOL MODEL SYSTEM

Problem Variable	Expected Maximum	$\frac{1}{\text{Expected Max.}}$	Scale Factor	Computer Variable
x_1	1.0	1.0	1.0	$[x_1]$
x_2	1.0	1.0	1.0	$[x_2]$
x_3	1.0	1.0	1.0	$[x_3]$
x_D	1.0	1.0	1.0	$[x_D]$

$$[x_D] = 0.22[x_1] + 0.22\,[x_2] + 0.56$$

The time scale factor was again taken as unity. The scaled circuit diagrams for the mixing pool model system is shown in Figure A-2.

3. DIGITAL COMPUTER SOLUTION OF THE REFERENCE SYSTEM.

The canonical equations of the reference system comprising of equations (11), (14), (16) and (17), were solved along with the boundary conditions of equation (21a) by a trial and error method outlined in Figure 5. The various symbols used in the program are explained in Table A-3 and a sample program is given in Table A-4.

4. DIGITAL COMPUTER SOLUTION OF THE MIXING POOL MODEL SYSTEM.

Due to the singular nature of the control policy for the mixing pool model system, the sampled data method of Grethlein and Lapidus was applied to the system equations (32). The symbols used in the digital computer program according to Figure 36 are explained in Table A-5 and a sample program is given in Table A-6. This program had to be run by double precision due to the very small numbers that were involved in the computations.

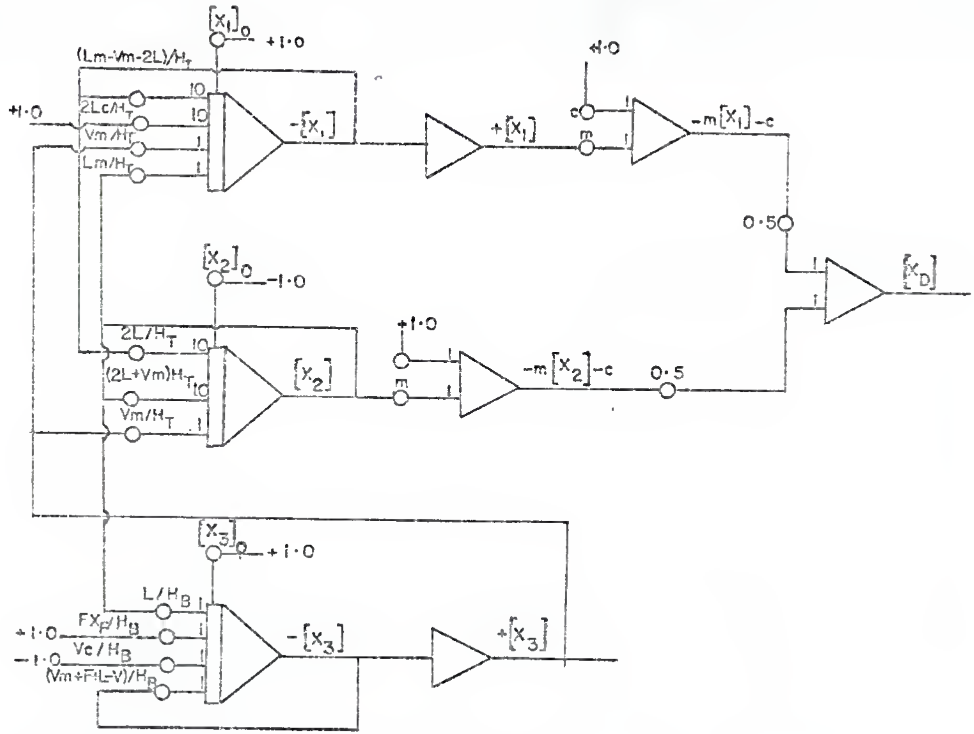


Fig. A-2. Analog computer circuit diagram for equations (A-4).

TABLE A-3. NOMENCLATURE FOR TRIAL AND ERROR SOLUTION OF MAXIMUM PRINCIPLE EQUATIONS.

Program Symbol	Designation
A	Switching function
AL	Control variable L
AUX	Auxiliary storage array
DERY (NDIM)	The differential equations that are integrated by subroutine RKGS
FCT	Name of external subroutine which defines the differential equations DERY (NDIM)
H	Hamiltonian
NDIM	Number of differential equations to be integrated by subroutine RKGS
OUTP	Name of external subroutine for handling output from subroutine RKGS
PRMT (1)	Initial time of integration
PRMT (2)	Final time of integration
PRMT (3)	Increment of independent variable t, over which integration is performed
PRMT (4)	Tolerated error
PRMT (5)	Parameter used to terminate subroutine RKGS at any desired output point
Q	Decimal counter used to monitor the printing of results at various points in time. Initially Q is zero and after integration commences Q is incremented by 0.01 each time results are printed
X	Independent variable t
Y(I)	Dependent variable x

TABLE A-4. COMPUTER PROGRAM FOR TRIAL AND ERROR SOLUTION OF MAXIMUM PRINCIPLE EQUATIONS

```
      EXTERNAL FCT,OUTP
      DIMENSION PRMT(5),Y(3),DERY(3),AUX(8,3)
      COMMON AL,Q
    4 FORMAT(1H ,6HIHLF =,I3)
      PRMT(1)=0.
      PRMT(2)=4.
      PRMT(3)=.01
      PRMT(4)=.0001
      AL=1.333
      Q=0.0
      NDIM=5
      DERY(1)=NDIM
      DERY(1)=1.E0/DERY(1)
      DO 7 I=2,NDIM
    7 DERY(I)=DERY(1)
      Y(1)=0.6300
      Y(2)=.2767
      Y(3)=0.0
      Y(5)=-.03
      Y(4)=-(1.+(.1413*AL-.1213)*Y(5))/(.2071*AL-.2071)
      CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      IF(IHLF.GT.10)WRITE(3,4)IHLF
      CONTINUE
   12 STOP
      END
```

TABLE A-4. (CONT.)

```
      SUBROUTINE FCT(X,Y,DERY)
      DIMENSION Y(1),DERY(1)
      COMMON AL,Q
      DERY(1)=.44*AL*Y(1)-.5865*Y(1)-AL*Y(1)+.5865*Y(2)+.56*AL
      DERY(2)=.4*AL*Y(1)+.0986*Y(2)-.4*AL*Y(2)-0.1486
      DERY(3)=1.
      DERY(4)=-.44*AL*Y(4)+.5865*Y(4)+AL*Y(4)+.4*AL*Y(5)
      DERY(5)=-.5865*Y(4)-.0986*Y(5)+.4*AL*Y(5)
      RETURN
      END
```

```
      SUBROUTINE OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
      DIMENSION PRMT(1),Y(1),DERY(1)
      COMMON AL,Q
   20 FORMAT(5X,F6.3)
   15 FORMAT(1X,4H T =,E11.4,6HX(1) =,E11.4,6HX(2) =,E11.4,6HX(3) =
     11.4,6HZ(1) =,E11.4,6HZ(2) =,E11.4,4HL =,F6.3)
      IF(X-Q) 99,16,16
   16 WRITE(3,15)X,(Y(I),I=1,5),AL
      A=.44*Y(1)*Y(4)-Y(1)*Y(4)+.56*Y(4)+.4*Y(1)*Y(5)-.4*Y(2)*Y(5)
      IF(A) 17,17,18
   17 AL=1.333
      GO TO 101
  18  AL=.833
  101 Q=Q+0.01
      H=(.44*AL*Y(1)-.5865*Y(1)-AL*Y(1)+.5865*Y(2)+.56*AL)*Y(4)
     1+(.4*AL*Y(1)+.0986*Y(2)-.4*AL*Y(2)-.1486)*Y(5)+1.
      WRITE (3,20) H
      GO TO 99
   9  PRMT(5)=1.0
   99 RETURN
      END
```

TABLE A-4. (CONT.)

```
      SUBROUTINE RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      DIMENSION Y(1),DERY(1),AUX(8,1),A(4),B(4),C(4),PRMT(1)
      DO 1 I=1,NDIM
    1 AUX(8,I)=.06666667*DERY(I)
      X=PRMT(1)
      XEND=PRMT(2)
      H=PRMT(3)
      PRMT(5)=0.
      CALL FCT(X,Y,DERY)
C
C     ERROR TEST
      IF(H*(XEND-X))38,37,2
C
C     PREPARATIONS FOR RUNGE-KUTTA METHOD
    2 A(1)=.5
      A(2)=.2928932
      A(3)=1.707107
      A(4)=.1666667
      B(1)=2.
      B(2)=1.
      B(3)=1.
      B(4)=2.
      C(1)=.5
      C(2)=.2928932
      C(3)=1.707107
      C(4)=.5
C
C     PREPARATIONS OF FIRST RUNGE-KUTTA STEP
      DO 3 I=1,NDIM
      AUX(1,I)=Y(I)
      AUX(2,I)=DERY(I)
      AUX(3,I)=0.
    3 AUX(6,I)=0.
      IREC=0
      H=H+H
      IHLF=-1
      ISTEP=0
      IEND=0
C
C
C     START OF A RUNGE-KUTTA STEP
    4 IF((X+H-XEND)*H)7,6,5
    5 H=XEND-X
    6 IEND=1
C
C     RECORDING OF INITIAL VALUES OF THIS STEP
    7 CALL OUTP(X,Y,DERY,IREC,NDIM,PRMT)
      IF(PRMT(5))40,8,40
    8 ITEST=0
    9 ISTEP=ISTEP+1
```

TABLE A-4. (CONT.)

```
C
C
C     START OF INNERMOST RUNGE-KUTTA LOOP
      J=1
   10 AJ=A(J)
      BJ=B(J)
      CJ=C(J)
      DO 11 I=1,NDIM
      R1=H*DERY(I)
      R2=AJ*(R1-BJ*AUX(6,I))
      Y(I)=Y(I)+R2
      R2=R2+R2+R2
   11 AUX(6,I)=AUX(6,I)+R2-CJ*R1
      IF(J-4)12,15,15
   12 J=J+1
      IF(J-3)13,14,13
   13 X=X+.5*H
   14 CALL FCT(X,Y,DERY)
      GOTO 10
C     END OF INNERMOST RUNGE-KUTTA LOOP
C
C
C     TEST OF ACCURACY
   15 IF(ITEST)16,16,20
C
C     IN CASE ITEST=0 THERE IS NO POSSIBILITY FOR TESTING OF ACCURA
   16 DO 17 I=1,NDIM
   17 AUX(4,I)=Y(I)
      ITEST=1
      ISTEP=ISTEP+ISTEP-2
   18 IHLF=IHLF+1
      X=X-H
      H=.5*H
      DO 19 I=1,NDIM
      Y(I)=AUX(1,I)
      DERY(I)=AUX(2,I)
   19 AUX(6,I)=AUX(3,I)
      GOTO 9
C
C     IN CASE ITEST=1 TESTING OF ACCURACY IS POSSIBLE
   20 IMOD=ISTEP/2
      IF(ISTEP-IMOD-IMOD)21,23,21
   21 CALL FCT(X,Y,DERY)
      DO 22 I=1,NDIM
      AUX(5,I)=Y(I)
   22 AUX(7,I)=DERY(I)
      GOTO 9
C
C     COMPUTATION OF TEST VALUE DELT
   23 DELT=0.
```

TABLE A-4. (CONT.)

```
      DO 24 I=1,NDIM
   24 DELT=DELT+AUX(8,I)*ABS(AUX(4,I)-Y(I))
      IF(DELT-PRMT(4))28,28,25
C
C     ERROR IS TOO GREAT
   25 IF(IHLF-10)26,36,36
   26 DO 27 I=1,NDIM
   27 AUX(4,I)=AUX(5,I)
      ISTEP=ISTEP+ISTEP-4
      X=X-H
      IEND=0
      GOTO 18
C
C     RESULT VALUES ARE GOOD
   28 CALL FCT(X,Y,DERY)
      DO 29 I=1,NDIM
      AUX(1,I)=Y(I)
      AUX(2,I)=DERY(I)
      AUX(3,I)=AUX(6,I)
      Y(I)=AUX(5,I)
   29 DERY(I)=AUX(7,I)
      CALL OUTP(X-H,Y,DERY,IHLF,NDIM,PRMT)
      IF(PRMT(5))40,30,40
   30 DO 31 I=1,NDIM
      Y(I)=AUX(1,I)
   31 DERY(I)=AUX(2,I)
      IREC=IHLF
      IF(IEND)32,32,39
C
C     INCREMENT GETS DOUBLED
   32 IHLF=IHLF-1
      ISTEP=ISTEP/2
      H=H+H
      IF(IHLF)4,33,33
   33 IMOD=ISTEP/2
      IF(ISTEP-IMOD-IMOD)4,34,4
   34 IF(DELT-.02*PRMT(4))35,35,4
   35 IHLF=IHLF-1
      ISTEP=ISTEP/2
      H=H+H
      GOTO 4
C
C
C     RETURNS TO CALLING PROGRAM
   36 IHLF=11
      CALL FCT(X,Y,DERY)
      GOTO 39
   37 IHLF=12
      GOTO 39
   38 IHLF=13
```

TABLE A-4. (CONT.)

```
39 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
40 RETURN
   END
```

TABLE A-5. NOMENCLATURE FOR THE SAMPLED DATA METHOD OF GRETHLEIN AND LAPIDUS

Program Symbol	Designation
AL(J)	Array containing five values of control variable L with values between L_{max} and L_{min}
AP	Control variable L used in conjunction with the differential equations
ALEM	Minimizing decision variable L from among the 5 specified in AL(J)
DERY (NDIM)	The differential equations that are integrated by subroutine RKGS
DEV(J)	Deviations corresponding to the control variables from array AL(J)
FCT	External subroutine wherein the differential equations DERY (NDIM) are defined
N	Number of current sampling period
NN	Total number of sampling periods
NDIM	Number of differential equations to be integrated by subroutine RKGS
OUTP	External subroutine used for purposes of handling output from subroutine RKGS
PRMT (1)	Initial time of integration of current sampling period
PRMT (2)	Final time of integration of current sampling period
PRMT (3)	Increment of independent variable t, over which integration is performed
PRMT (4)	Tolerated error
PRMT (5)	Parameter used for terminating subroutine RKGS at any desired output point

TABLE A-5. (CONT.)

Program Symbol	Designation
Q	Decimal counter used to ensure the completion of integration over entire sampling period before evaluating DEV(J)
SUM	Value of deviation computed from objective function before being stored into DEV(J)
SUMT	Summation of minimum deviations over all sampling periods upto and including present sampling period
X	Independent variable t
Y(I)	Dependent variables $\dot{x}$

TABLE A-6. COMPUTER PROGRAM FOR THE SAMPLED DATA METHOD OF GRETHLEIN AND LAPIDUS

```
      IMPLICIT REAL*8(A-H,O-Z)
      EXTERNAL FCT,OUTP
C
C
      DIMENSION PRMT(6),Y(4),DERY(4),AUX(8,4),YS(3),AL(10),DEV(5)
      COMMON AP,N,YS,J,M,II,ALEM,YA,YB,YC,YD,AL,SUMT
C
C     READ NUMERICAL DATA ****************************************
C
      NDIM=4
      PRMT(1)=0.0
      PRMT(2)=0.05
      PRMT(3)=0.010
      PRMT(4)=0.1
      YS(1)=0.71399
      YS(2)=0.60986
      YS(3)=0.28247
      AL(1)=.833
      AL(2)=.958
      AL(3)=1.083
      AL(4)=1.208
      AL(5)=1.333
      N=1
      NN=250
      II=1
      M=0
      SUMT=0.0
C
C
C     READ PARAMETERS FOR ITERATION WITH AL(1) ******************
C
  100 J=1
      AP=AL(J)
      IF(M.EQ.1) GO TO 150
      Y(1)=0.71467
      Y(2)=0.60909
      Y(3)=0.24899
      Y(4)=0.0
      GO TO 101
  150 Y(1)=YA
      Y(2)=YB
      Y(3)=YC
      Y(4)=YD
  101 CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      CONTINUE
C
C     READ PARAMETERS FOR ITERATION WITH AL(2) ******************
C
      AP=AL(J)
      IF(M.EQ.1) GO TO 160
```

```
      Y(1)=0.71467
      Y(2)=0.60909
      Y(3)=0.24899
      Y(4)=0.0
      GO TC 102
  160 Y(1)=YA
      Y(2)=YB
      Y(3)=YC
      Y(4)=YD
  102 CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      CONTINUE
C
C     READ PARAMETERS FOR ITERATION WITH AL(3) ******************
C
      AP=AL(J)
      IF(M.EQ.1) GO TO 170
      Y(1)=0.71467
      Y(2)=C.60909
      Y(3)=0.24899
      Y(4)=0.0
      GO TC 103
  170 Y(1)=YA
      Y(2)=YB
      Y(3)=YC
      Y(4)=YD
  103 CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      CONTINUE
C
C     READ PARAMETERS FOR ITERATION WITH AL(4) ******************
C
      AP=AL(J)
      IF(M.EQ.1) GO TO 180
      Y(1)=C.71467
      Y(2)=0.60909
      Y(3)=0.24899
      Y(4)=C.0
      GO TC 104
  180 Y(1)=YA
      Y(2)=YB
      Y(3)=YC
      Y(4)=YD
  104 CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      CONTINUE
C
C     READ PARAMETERS FOR ITERATION WITH AL(5) ******************
C
      AP=AL(J)
      IF(M.EQ.1) GO TO 190
      Y(I)=0.71467
      Y(2)=0.60909
```

TABLE A-6. (CONT.)

```
      Y(3)=0.24899
      Y(4)=0.0
      GO TO 105
  190 Y(1)=YA
      Y(2)=YB
      Y(3)=YC
      Y(4)=YD
  105 CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      CONTINUE
C
C     READ PARAMETERS FOR ITERATION WITH ALEM  *******************
C
      AP=ALEM
      IF(M.EQ.1) GO TO 200
      Y(1)=0.71467
      Y(2)=0.60909
      Y(3)=0.24899
      Y(4)=0.0
      GO TO 106
  200 Y(1)=YA
      Y(2)=YB
      Y(3)=YC
      Y(4)=YD
  106 CALL RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      CONTINUE
C
C     RETURN FOR REITERATION AT (N+1)TH SAMPLING PERIOD***********
C
      I1=1
      M=1
      N=N+1
      AN=N-1
      Y(1)=YA
      Y(2)=YB
      Y(3)=YC
      Y(4)=YD
      PRMT(1)=AN*0.05
      PRMT(2)=PRMT(1)+0.05
      IF(N.LE.NN) GO TO 100
      STOP
      END
```

TABLE A-6. (CONT.)

```
      SUBROUTINE RKGS(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)
      IMPLICIT REAL*8(A-H,O-Z)
C
C
      DIMENSION Y(1),DERY(1),AUX(8,1),A(4),B(4),C(4),PRMT(1)
      X=PRMT(1)
      H=PRMT(3)
      PRMT(5)=0.
      CALL FCT(X,Y,DERY)
C
C
C     PREPARATIONS FOR RUNGE-KUTTA METHOD
    2 A(1)=.5
      A(2)=.2928932
      A(3)=1.707107
      A(4)=.1666667
      B(1)=2.
      B(2)=1.
      B(3)=1.
      B(4)=2.
      C(1)=.5
      C(2)=.2928932
      C(3)=1.707107
      C(4)=.5
C
C     PREPARATIONS OF FIRST RUNGE-KUTTA STEP
      DO 3 I=1,NDIM
      AUX(1,I)=Y(I)
      AUX(2,I)=DERY(I)
      AUX(3,I)=0.
    3 AUX(6,I)=0.
C
C     RECORDING OF INITIAL VALUES OF THIS STEP
    7 CALL OUTP(X,Y,DERY,IREC,NDIM,PRMT)
      IF(PRMT(5))40,8,40
C
C
C     START OF INNERMOST RUNGE-KUTTA LOOP
    8 J=1
   10 AJ=A(J)
      BJ=B(J)
      CJ=C(J)
      DO 11 I=1,NDIM
      R1=H*DERY(I)
      R2=AJ*(R1-BJ*AUX(6,I))
      Y(I)=Y(I)+R2
      R2=R2+R2+R2
   11 AUX(6,I)=AUX(6,I)+R2-CJ*R1
      IF(J-4)12,15,15
   12 J=J+1
```

TABLE A-6. (CONT.)

```
      IF(J-3)13,14,13
   13 X=X+.5*H
   14 CALL FCT(X,Y,DERY)
      GOTO 10
C     END OF INNERMOST RUNGE-KUTTA LOOP
C
C
   15 DO 29 I=1,NDIM
      AUX(1,I)=Y(I)
      AUX(2,I)=DERY(I)
   29 AUX(6,I)=AUX(3,I)
      CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
      IF(PRMT(5))40,30,40
   30 DO 31 I=1,NDIM
      Y(I)=AUX(1,I)
   31 DERY(I)=AUX(2,I)
      GO TO 8
   40 RETURN
      END
```

```
      SUBROUTINE FCT(X,Y,DERY)
      IMPLICIT REAL*8(A-H,O-Z)
C
C
      DIMENSION Y(4),DERY(4),YS(3),AL(10)
      COMMON AP,N,YS,J,M,II,ALEM,YA,YB,YC,YD,AL,SUMT
C
C     DEFINE DIFFERENTIAL EQUATIONS  ******************************
C
      DERY(1)=-1.56*AP*Y(1)-.58652*Y(1)+.44*AP*Y(2)+.58652*Y(3)+1.1
      DERY(2)=2.0*AP*Y(1)-.58652*Y(2)-2.0*AP*Y(2)+.58652*Y(3)
      DERY(3)=AP*.4*Y(2)+0.0986*Y(3)-0.4*AP*Y(3)-0.148592
      DERY(4)=(.85123-.22*Y(1)-.22*Y(2)-.56)*
     1(.85123-.22*Y(1)-.22*Y(2)-.56)
      RETURN
      END
```

TABLE A-6. (CONT.)

```
      SUBRCUTINF OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
      IMPLICIT REAL*8(A-H,O-Z)
C
C
      DIMENSION PRMT(6),Y(4),DERY(4),YS(3),AL(10),DEV(5)
      COMMCN AP,N,YS,J,M,II,ALEM,YA,YB,YC,YD,AL,SUMT
    1 FORMAT(5X,4HDEV(,I1,4H) = ,F14.8)
    2 FORMAT(5X,4HN = ,I3)
    3 FORMAT(5X,5HAP = ,F10.5)
    4 FORMAT(5X,7HX(1) = ,F10.5,5X,7HX(2) = ,F10.5,5X,7HX(3) = ,F10
     15X,7HX(4) = ,F14.9)
    5 FORMAT(5X,7HDEVM = ,F14.8)
  111 BN=N
      Q=BN*C.05
      IF(X-Q) 20,10,10
   20 RETURN
   10 IF(II.LE.0) GO TO 50
C
C     CALCULATE DEVIATIONS FROM STEADY STATE FOR JTH REFLUX RATE****
C
      SUM=SUMT+
     1                                 (.28247-Y(3))*(.28247-Y(3))
      DEV(J)=SUM
      WRITE(3,1) J, DEV(J)
      IF(J.GE.5) GO TO 30
      J=J+1
      PRMT(5)=1.0
      RETURN
C
C     FIND MINIMUM DEVIATION  ************************************
C
   30 DMIN=DEV(1)
      JMIN=1
      DO 40 J=2,5
      IF(DEV(J).LT.DMIN) JMIN=J
      IF(DEV(J).LT.DMIN) DMIN=DEV(J)
   40 CONTINUE
      AL1=AL(1)
      AL2=AL(2)
      AL3=AL(3)
      AL4=AL(4)
      AL5=AL(5)
      DEV1=DEV(1)
      DEV2=DEV(2)
      DEV3=DEV(3)
      DEV4=DEV(4)
      DEV5=DEV(5)
      IF(JMIN.EQ.1) ALFM=AL(JMIN)
      IF(JMIN.EQ.1) WRITE(3,5)DEV(JMIN)
      IF(JMIN.EQ.1) DEVJ=DEV(JMIN)
```

TABLE A-6. (CONT.)

```
      IF(JMIN.EQ.5) ALEM=AL(JMIN)
      IF(JMIN.EQ.5) WRITE(3,5)DEV(JMIN)
      IF(JMIN.EQ.5) DEVJ=DEV(JMIN)
      IF(JMIN.EQ.2) CALL POLI(DEV1,DEV2,DEV3,AL1,AL2,AL3,ALEM,DEVJ
      IF(JMIN.EQ.3) CALL POLI(DEV2,DEV3,DEV4,AL2,AL3,AL4,ALEM,DEVJ
      IF(JMIN.EQ.4) CALL POLI(DEV3,DEV4,DEV5,AL3,AL4,AL5,ALEM,DEVJ
      AP=ALEM
      SUMT=DEVJ
      II=0
      PRMT(5)=1.0
      RETURN
C
C     WRITE SOLUTIONS FOR NTH SAMPLING PERIOD*******************
C
   50 WRITE(3,2) N
      WRITE(3,3) AP
      WRITE(3,4) Y(1),Y(2),Y(3),Y(4)
      YA=Y(1)
      YB=Y(2)
      YC=Y(3)
      YD=Y(4)
      PRMT(5)=1.0
      RETURN
      END
```

```
      SUBROUTINE POLI(F1,F2,F3,R1,R2,R3,RMIN,FMIN)
      IMPLICIT REAL*8(A-H,O-Z)
  200 FORMAT(5X,7HRMIN = ,F10.5,5X,7HDEVM = ,F14.8)
C
C     CALCULATE COEFFCIENTS OF 3 POINT LAGRANGIAN****************
C
  112 D1=(R1-R2)*(R1-R3)
      D2=(R2-R1)*(R2-R3)
      D3=(R3-R1)*(R3-R2)
      E1=F1/D1
```

TABLE A-6. (CONT.)

```
      E2=F2/D2
      E3=F3/D3
      G1=R2+R3
      G2=R1+R3
      G3=R1+R2
      H1=R2*R3
      H2=R1*R3
      H3=R1*R2
      A=E1+E2+E3
      B=E1*G1+E2*G2+E3*G3
      C=E1*H1+E2*H2+E3*H3
C
C     CALCULATE RMIN AND FMIN
C
      RMIN=B/(2.0*A)
      FMIN=A*RMIN*RMIN-B*RMIN+C
      WRITE(3,200) RMIN,FMIN
      RETURN
      END
```

APPENDIX B

STEADY STATE AND LIMITING CASE ANALYSES

In order to determine the physically realizable bounds of the two systems studied in this work, steady state and limiting case analyses have been carried out for each system. This Appendix deals with these analyses starting with the reference system analysis.

1. REFERENCE SYSTEM ANALYSIS.

The performance equations of the reference system are

$$\frac{dx_1}{dt} = \frac{(Lm - Vm - L)}{H_T} x_1 + \frac{Vm}{H_T} x_2 + \frac{Lc}{H_T} \tag{B-1}$$

$$\frac{dx_2}{dt} = \frac{L}{H_B} x_1 - \frac{(Vm + F + L - V)}{H_B} x_2 + \frac{Fx_F}{H_B} - \frac{Vc}{H_B} \tag{B-2}$$

Multiplying equations (B-1) and (B-2) by H_T and H_B respectively, and setting the derivatives with respect to time, of the resulting equations, equal to zero yields

$$(Lm - Vm - L)x_1 + Vm\ x_2 = - Lc \tag{B-3}$$

$$L\ x_1 - (Vm + B)x_2 = Vc - Fx_F \tag{B-4}$$

which can be put in matrix form as

$$\begin{bmatrix} Lm - Vm - L & Vm \\ L & -(Vm + B) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -Lc \\ Vc - Fx_F \end{bmatrix} \tag{B-5}$$

Equation (B-5) is of the form

$$AX = B \tag{B-6}$$

from which X can be solved for uniquely by applying Cramer's Rule, provided the coefficient matrix A is nonsingular. Hence, the system has the unique solution

$$x_1 = \frac{\begin{vmatrix} -Lc & Vm \\ Vc - Fx_F & -(Vm + B) \end{vmatrix}}{\begin{vmatrix} Lm - Vm - L & Vm \\ L & -(Vm + B) \end{vmatrix}} \tag{B-7}$$

and

$$x_2 = \frac{\begin{vmatrix} Lm - Vm - L & -Lc \\ L & Vc - Fx_F \end{vmatrix}}{\begin{vmatrix} Lm - Vm - L & Vm \\ L & -(Vm + B) \end{vmatrix}} \tag{b-8}$$

Equations (B-7) and (B-8) can be further simplified to

$$x_1 = \frac{LVmc + BLc - V^2mc + FVmx_F}{V^2m^2 - LVm^2 + BVm - BLm + BL} \tag{B-9}$$

and

$$x_2 = \frac{LVmc - V^2mc - LVc - FLmx_F + FVmx_F + FLx_F + L^2c}{V^2m^2 - LVm^2 + BVm - BLm + BL} \tag{B-10}$$

Hence x_1 and x_2 can be generally written as

$$x_1 = x_1(L,\ V,\ F,\ B,\ m,\ c,\ x_F)$$
$$x_2 = x_2(L,\ V,\ F,\ B,\ m,\ c,\ x_F) \qquad \text{(B-11)}$$

however, m and c are fixed by the equilibrium relation of equation (4a)

$$y_i = 0.44\ x_i + 0.56 \qquad i = 1,\ 2$$

and B is itself a function F, V and L as can be seen in equation (1a),

$$B = F + L - V$$

whereby

$$x_1 = x_1(L,\ V,\ F,\ x_F)$$
$$x_2 = x_2(L,\ V,\ F,\ x_F) \qquad \text{(B-12)}$$

Thus x_1 and x_2 have been reduced to being dependent on the four parameters L, V, F and x_F. It is obvious that for each set of values for the above parameters, x_1 and x_2 have unique values corresponding to a unique steady state; and also innumerable combinations of the above parameters will give rise to innumerable steady states. Hence, in order to narrow down the range of steady state solutions of the reference system, we shall restrict ourselves to the case where V, F, and x_F are held constant as prescribed by equation (4), i.e.

$$V = 1.333 \text{ lb. moles/min.}$$
$$F = 0.5 \text{ lb. moles/min.} \qquad \text{(B-13)}$$

$$x_F = 0.65 \qquad \text{(B-13 cont.)}$$

Utilizing the overall material balance and a material balance around the reflux drum, we have

$$F = D + B$$

and

$$V = L + D$$

respectively; and using the values of V and F as in equation (B-13) we find that L is restricted to values between 0.833 and 1.333. Physically this means that the overhead reflus flow rate can be varied from a minimum of 0.833 lb. moles/min. to a maximum of 1.333 lb. moles/min.

The steady state analysis consists of using values of V, F and x_F given by equation (B-13), in equations (B-9) and (B-10) and evaluating x_1 and x_2 as L is varied between its lower and upper limits. This same procedure is then repeated for different values of x_F (since ultimately we wish to determine an optimal path for L so as to counteract a known disturbance in x_F).

The results are plotted in figure B-1, for $x_F = 0.55$, 0.65, and 0.75. Also in the plot are included curves for the overhead composition x_D since

$$x_D = y_1 = mx_1 + c$$

Figure B-1 acts as an aid in determining the range within which the reference system can operate for the given set of parameters.

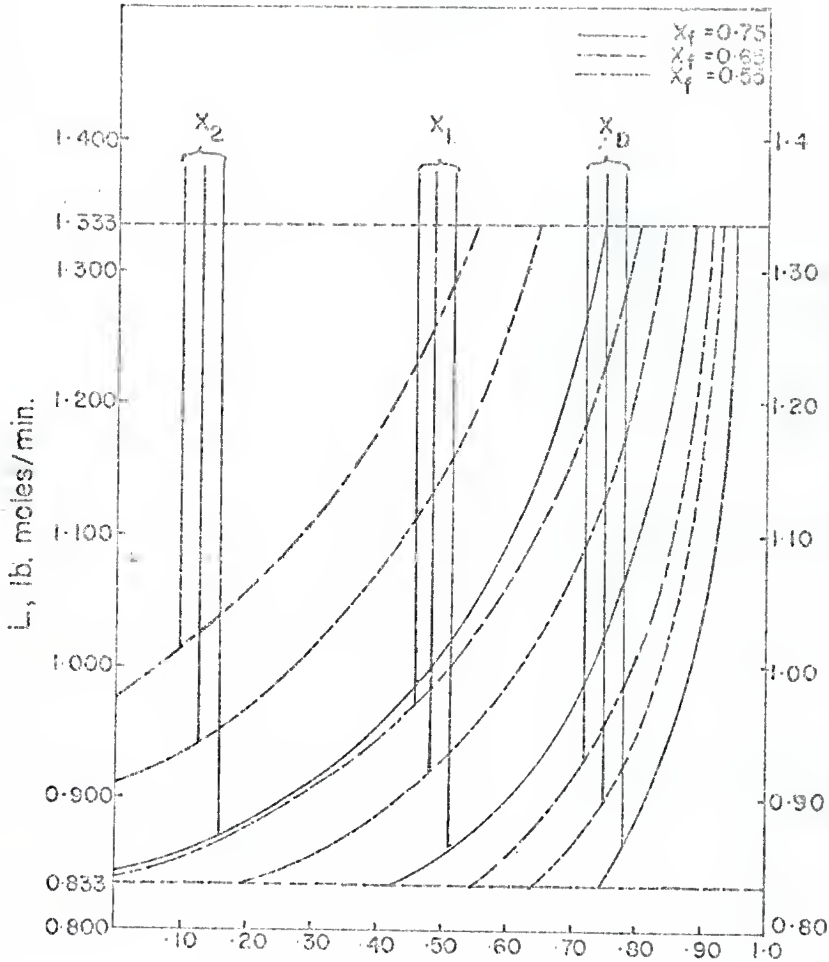


Fig. B-1. L V/s X with X_f as parameter for reference system.

2. MIXING POOL MODEL SYSTEM ANALYSIS

The performance equations of the mixing pool model are,

$$\frac{dx_1}{dt} = \frac{(Lm - Vm - 2L)}{H_T} x_1 + \frac{Lm}{H_T} x_2 + \frac{Vm}{H_T} x_3 + \frac{2Lc}{H_T} \qquad \text{(B-14)}$$

$$\frac{dx_2}{dt} = \frac{2L}{H_T} x_1 - \frac{(Vm + 2L)}{H_T} x_2 + \frac{Vm}{H_T} x_3 \qquad \text{(B-15)}$$

$$\frac{dx_3}{dt} = \frac{L}{H_B} x_2 - \frac{(Vm + F + L - V)}{H_B} x_3 + \frac{Fx_F}{H_B} - \frac{Vc}{H_B} \qquad \text{(B-16)}$$

Multiplying equations (B-14) and (B-15) by H_T and equation (B-16) by H_B and setting the time derivatives in the resulting equations equal to zero gives

$$(Lm - 2L - Vm)x_1 + Lmx_2 + Vmx_3 = -2Lc \qquad \text{(B-17)}$$

$$2Lx_1 - (Vm + 2L)x_2 + Vmx_3 = 0 \qquad \text{(B-18)}$$

$$Lx_2 - (Vm + F + L - V)x_3 = Vc - Fx_F \qquad \text{(B-19)}$$

which in matrix form becomes

$$\begin{bmatrix} Lm - 2L - Vm & Lm & Vm \\ 2L & -(Vm + 2L) & Vm \\ 0 & & -(Vm + F + L - V) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$= \begin{bmatrix} -2Lc \\ 0 \\ Vc - Fx_F \end{bmatrix} \qquad \text{(B-20)}$$

Again, equation (B-20) is of the form

$$AX = B$$

from which X can be solved for by using Cramer's Rule, provided the coefficient matrix A is nonsingular. Hence, the unique solution of the system is

$$x_1 = \frac{\begin{vmatrix} -2Lc & Lm & Vm \\ 0 & -(2L+Vm) & Vm \\ Vc-Fx_F & L & -(Vm+F+L-V) \end{vmatrix}}{A} \tag{B-21}$$

$$x_2 = \frac{\begin{vmatrix} Lm-Vm-2L & -2Lc & Vm \\ 2L & 0 & Vm \\ 0 & Vc-Fx_F & -(Vm+F+L-V) \end{vmatrix}}{A} \tag{B-22}$$

and

$$x_3 = \frac{\begin{vmatrix} Lm-Vm-2L & Lm & -2Lc \\ 2L & -(2L+Vm) & 0 \\ 0 & L & Vc-Fx_F \end{vmatrix}}{A} \tag{B-23}$$

where

$$A = \begin{vmatrix} Lm-2L-Vm & Lm & Vm \\ 2L & -(Vm+2L) & Vm \\ 0 & L & -(Vm+F+L-V) \end{vmatrix}$$

Equations (B-21), (B-22), and (B-23) can be further simplified to

$$x_1 = \frac{N_1}{D} \tag{B-24}$$

where

$$N_1 = -4cL^3 - 4FcL^2 + (4c - 4mc)L^2V - (2Fmc + Fm^2x_F + 2Fmx_F)$$
$$LV + (4mc - m^2c)LV^2 - Fm^2x_FV^2 + m^2cV^3$$

and

$$D = (4m - 4)L^3 + (4Fm - 4F)L^2 + (4m^2 - 8m + 4)L^2V$$
$$+ (Fm^2 - 4Fm)LV + (4m - 5m^2 + m^3)LV^2 - Fm^2V^2 - (m^3 - m^3)V^3$$

$$x_2 = \frac{N_2}{D} \tag{B-25}$$

where

$$N_2 = -4cL^3 - 4FcL^2 + (4c - 4mc)L^2V + (Fx_Fm^2 - 4Fx_Fm)LV$$
$$+ (4mc - m^2c)LV^2 - Fx_Fm^2V^2 + m^2cV^3$$

and

$$x_3 = \frac{N_3}{D} \tag{B-26}$$

where

$$N_3 = -4cL^3 + (4Fx_Fm - 4Fx_F)L^2 + (4c - 4mc)L^2V$$
$$+ (Fx_Fm^2 - 4Fx_Fm)LV + (4mc - m^2c)LV^2 - Fm^2x_FV^2 + m^2cV^3$$

Hence, x_1, x_2 and x_3 can be generally written as

$$\begin{aligned} x_1 &= x_1(L, V, F, m, c, x_F) \\ x_2 &= x_2(L, V, F, m, c, x_F) \\ x_3 &= x_3(L, V, F, m, c, x_F) \end{aligned} \qquad \text{(B-27)}$$

which can be further reduced as in the reference system to

$$\begin{aligned} x_1 &= x_1(L, V, F, x_F) \\ x_2 &= x_2(L, V, F, x_F) \\ x_3 &= x_3(L, V, F, x_F) \end{aligned} \qquad \text{(B-28)}$$

Arguing along the same lines as in the reference system analysis, we have V, F, and x_F held constant as in equation (B-13) and find that L is restricted to taking on values between 0.833 and 1.333. Hence, the steady state analysis consists of holding V, F, and x_F constant in equations (B-24), (B-25) and (B-26) and evaluating x_1, x_2, and x_3 as L is varied between its lower and upper lomits; the procedure being repeated for different values of x_F.

The results are plotted in figure B-2 for $x_F = 0.55$, 0.65, and 0.75. Also in the plot are included curves for the overhead composition x_D since

$$x_D = 0.22(x_1 + x_2) + C$$

Figure B-2 acts as an aid in determining the range within which the mixing pool model can operate for the given set of parameters.

Diagrams of the type of figures B-1 and B-2 should form an integral part of any sort of analysis work involving systems

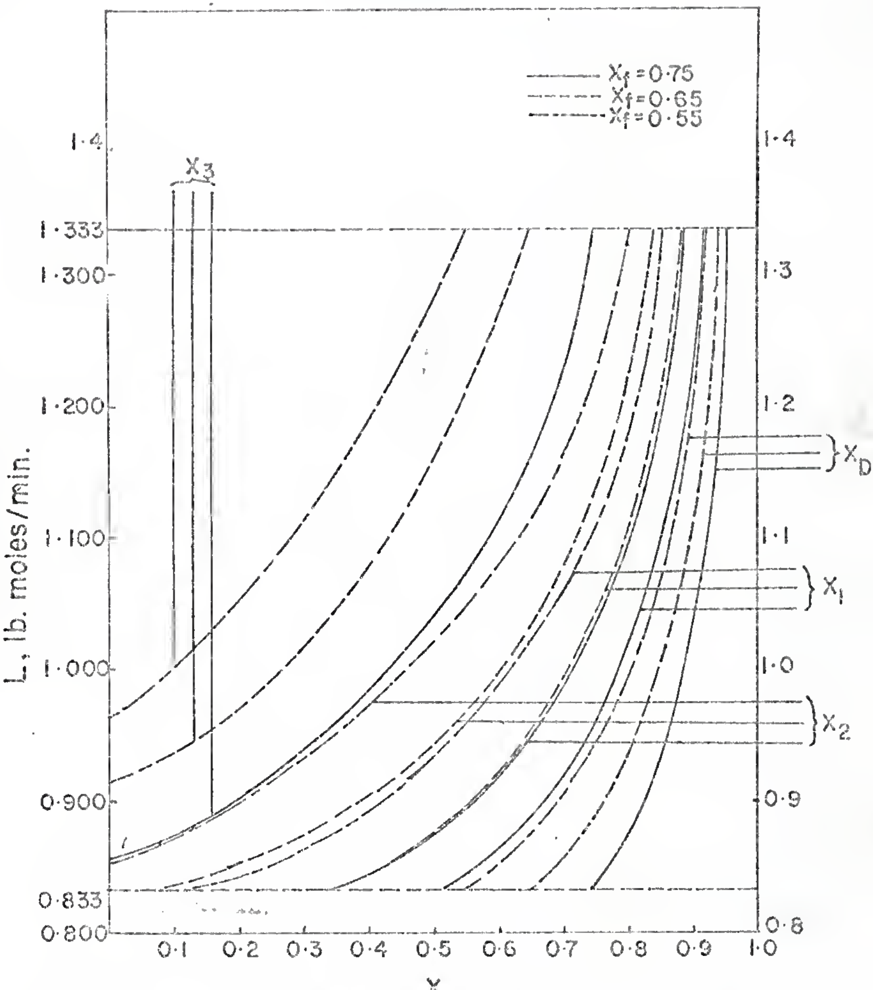


Fig. B-2. L V/s x for tanks-in-series model using x_f as parameter.

with several parameters since they give at a glance an overall picture of the limits within which the system operates.

APPENDIX C

COMPUTATIONAL ALGORITHM OF PONTRYAGIN'S MAXIMUM PRINCIPLE AND STATEMENTS OF THEOREMS ON EXISTENCE OF OPTIMAL CONTROLS

A continuous process is best represented by a set of simultaneous first-order differential equations; the number of equations depending on the order of the system. In general, an nth order continuous system can be represented by n simultaneous first order differential equations by using the concept of state space. The differential equations are called the performance equations of the process.

We shall now proceed to state the algorithm based on the Maximum Principle associated with continuous, autonomous (i.e. time does not appear explicitly) systems.

C-1. STATEMENT OF THE MAXIMUM PRINCIPLE ALGORITHM.

Let the performance equations of a process have the form

$$\frac{dx_i}{dt} = f_i(x_1(t), x_2(t), \ldots, x_n(t); \theta_1(t), \theta_2(t), \ldots, \theta_r(t)) \tag{C-1}$$

or the vector form

$$\frac{dx}{dt} = f(x(t); \theta(t)) \tag{C-2}$$

where $x(t)$ is an n-dimensional vector function representing the state of the process at time t and $\theta(t)$ is an r-dimensional vector function representing the decision at time t.

(In the case where the system is linear, the equation becomes

$$\frac{dx_i}{dt} = \sum_{j=1}^{n} a_{ij}\, x_j + \sum_{k=1}^{r} b_{ik}\, \theta_k) \tag{C-3}$$

with initial conditions

$$x_i(t)\Big|_{t=0} = x_i(0) = \alpha_i \qquad i = 1, 2, \ldots, n \tag{C-4}$$

The problem associated with such a process is to find or choose $\theta(t)$ subject to the constraint

$$\theta(t) \in \Phi \tag{C-5}$$

(where Φ is an r-dimensional space), which makes a function of the final values of the state

$$S = \sum_{i=1}^{n} C_i\, x_i(T), \qquad C_i = \text{const.} \tag{C-6}$$

a maximum (or a minimum). The function S to be extremized is called the objective function, and the decision vector function so chosen is called the optimal decision $\bar{\theta}(t)$.

The first step in solving such a problem is to introduce a new state variable so that the desired form of the objective function may be obtained. For example, if

$$S = \int_0^T (1 + \theta^2)dt$$

is the objective function, then an additional state variable x_{n+1} is introduced such that

$$x_{n+1}(T) = S = \int_0^T (1 + \theta^2)dt$$

or

$$\frac{dx_{n+1}}{dt} = 1 + \theta^2, \qquad x_{n+1}(0) = 0$$

and hence the objective function now becomes

$$S = x_{n+1}(T) \tag{C-7}$$

Finally an n-dimensional adjoint vector $z(t)$ is introduced along with a Hamiltonian function H which satisfy the following relations,

$$H(z(t), x(t), \theta(t) = \sum_{i=1}^{n} z_i \; f_i(x(t), \theta(t) \tag{C-8}$$

and

$$\frac{dz_i}{dt} = - \frac{\partial H}{\partial x_i} = - \sum_{j=1}^{n} z_j \frac{\partial f_j}{\partial x_i} \qquad i = 1, 2, \ldots, n \tag{C-9}$$

where

$$z_i(T) = C_i .$$

The set of equations (C-1) and (C-9) constitutes a split boundary value problem, whose solution depends on $\theta(t)$. The optimal decision vector function $\overline{\theta}(t)$ which makes S an extremum also makes the Hamiltonian an extremum for all t, $0 \leq t \leq T$. Furthermore, the maximum (or minimum) value of H is a constant for every t.

C-2. DERIVATION OF THE ALGORITHM

In this section we shall consider 3 basic types of problems and derive the Maximum Principle algorithm in each case. For the case where the final time is fixed we have two problems, a fixed right-hand and a free right-hand problem, depending on whether the final conditions on the state variables are given or not. The third problem arises for the case where the final time is left unfixed.

C-2.1. FINAL TIME FIXED AND FREE RIGHT-HAND PROBLEM

The system will be the same as governed by equations (C-1) and (C-4). The objective function is defined as in equation (C-6), and is to be maximized. Next the adjoint vector function along with the Hamiltonian is introduced as defined in equations (C-8) and (C-9).

Now, if $\bar{\theta}(t)$ represents the optimal decision vector such that S attains its maximum value, then a small perturbation $\delta\theta(t)$ will move the optimal state vector $\bar{x}(t)$ by a small deviation $\delta x(t)$, (see figure C-1). That is, if

$$\frac{d\bar{x}_i}{dt} = f_i(\bar{x}(t);\ \bar{\theta}(t)) \tag{C-10}$$

represents the optimal system, then after perturbation we have

$$\frac{d}{dt}\,(\bar{x}_i + \delta x_i) = f_i(\bar{x} + \delta x;\ \bar{\theta} + \delta\theta) \tag{C-11}$$

Upon subtracting equation (C-10) from equation (C-11) we have

$$\frac{d}{dt}\,\delta x_i = f_i(\bar{x} + \delta x;\ \bar{\theta} + \delta\theta) - f_i(\bar{x};\ \bar{\theta}) \tag{C-12}$$

Multiplying both sides by the adjoint variables $z_i(t)$ and then

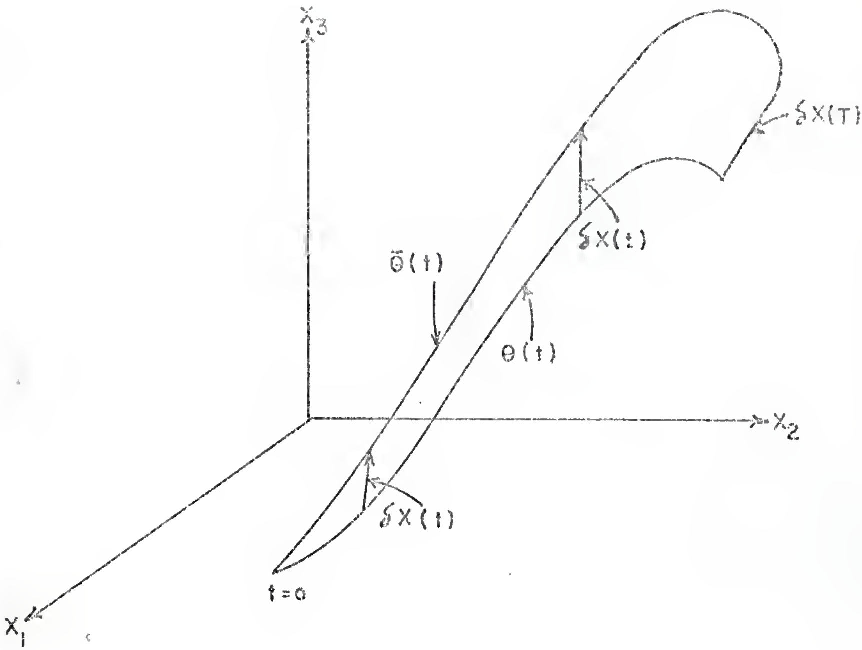


Fig. C-1. Perturbation trajectory due to change in decision variable for two dimensional system. Notice how $\delta x(0) = 0$ when initial values are preassigned.

taking the sum over the subscript i yields,

$$\sum_{i=1}^{n} z_i \frac{d}{dt}\delta x_i = \sum_{i=1}^{n} z_i \; f_i(\bar{x} + \delta x; \bar{\theta} + \delta\theta) - f_i(\bar{x}; \bar{\theta}) \qquad \text{(C-13)}$$

Next integrating both sides of equation (C-13) with respect to time from $t = 0$ to $t = T$ gives

$$\int_0^T \sum_{i=1}^{n} z_i \frac{d}{dt}\delta x_i dt = \int_0^T \sum_{i=1}^{n} z_i \; f_i(\bar{x} + \delta x; \bar{\theta} + \delta\theta) - f_i(\bar{x}; \bar{\theta}) dt \qquad \text{(C-14)}$$

Now consider the differentiation of $\sum_{i=1}^{n} z_i \; \delta x_i$

$$\frac{d}{dt} \sum_{i=1}^{n} z_i \; \delta x_i = \sum_{i=1}^{n} \frac{dx_i}{dt} \delta x_i + \sum_{i=1}^{n} z_i \frac{d}{dt} \delta x_i \qquad \text{(C-15)}$$

hence

$$\int_0^T \sum_{i=1}^{n} z_i \frac{d}{dt} \delta x_i dt = \sum_{i=1}^{n} z_i \delta x_i \Big|_0^T - \int_0^T \sum_{i=1}^{n} \frac{dz_i}{dt} \delta x_i dt \qquad \text{(C-16)}$$

Therefore combining equations (C-14) and (C-16) we get

$$\sum_{i=1}^{n} z_i \delta x_i \Big|_0^T = \int_0^T \sum_{i=1}^{n} \frac{dz_i}{dt} \delta x_i dt + \int_0^T \sum_{i=1}^{n} z_i \; f_i(\bar{x} + \delta x; \bar{\theta} + \delta\theta)$$
$$- f_i(\bar{x}; \bar{\theta}) dt \qquad \text{(C-17)}$$

Since the initial state values have been preassigned in equation (C-4)

$$\delta x_i(0) = 0 \qquad \text{(see figure C-1)}$$

and also since $z_i(T) = C_i$, we have

$$\sum_{n=1}^{n} z_i \; \delta x_i \Big|_0^T = \sum_{i=1}^{n} C_i \; \delta x_i(T) = \delta S, \qquad \text{(C-18)}$$

where δS represents the variation in the objective function.

From the Taylor Series expansion of a function about a point we have,

$$f(x_1, x_2, \ldots, x_n) = f(a_1, a_2, \ldots, a_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\Big|_{a_1, a_2, \ldots, a_n} (x_i - a_i) + \text{higher order terms}$$

where the second order partial derivatives are assumed to exist. Using this result, the factor within brackets in the second term on the right hand side of equation (C-17) becomes

$$\begin{aligned} & f_i(\bar{x} + \delta x;\ \bar{\theta} + \delta\theta) - f_i(\bar{x};\ \bar{\theta}) \\ &= f_i(\bar{x};\ \bar{\theta} + \delta\theta) - f_i(\bar{x};\ \bar{\theta}) + \sum_{j=1}^{n} \frac{\partial f_i}{\partial x_j}(\bar{x};\ \bar{\theta} + \delta\theta)\, \delta x_j \\ &\quad + \text{higher order terms} \end{aligned} \qquad \text{(C-19)}$$

Recalling equation (C-17) we have

$$\delta S = \int_0^T \sum_{i=1}^{n} \frac{dz_i}{dt} \delta x_i\, dt + \int_0^T \sum_{i=1}^{n} z_i [f_i(\bar{x} + \delta x;\ \bar{\theta} + \delta\theta) - f_i(\bar{x};\bar{\theta})] dt$$

and finally utilizing equations (C-9) and (C-19) gives

$$\delta S = -\int_0^T \sum_{i=1}^{n} \sum_{j=1}^{n} z_j \frac{\partial f_j}{\partial x_i} \delta x_i\, dt + \int_0^T \sum_{i=1}^{n} z_i [f_i(\bar{x}, + \delta\theta) - f_i(\bar{x};\bar{\theta})$$

$$+ \sum_{j=1}^{n} \frac{\partial f_i}{\partial x_j} (\bar{x};\ \bar{\theta} + \delta\theta) \delta x_j] dt$$

$$= \int_0^T \sum_{i=1}^{n} z_i [f_i(\bar{x};\ \bar{\theta} + \delta\theta) - f_i(\bar{x};\ \bar{\theta})] dt$$

$$+ \int_0^T \sum_{i=1}^n \sum_{j=1}^n z_i \frac{\partial f_i}{\partial x_j}(\bar{x};\bar{\theta}+\delta\theta) - \frac{\partial f_i}{\partial x_j}(\bar{x};\bar{\theta})\ \delta x_j dt \tag{C-20}$$

At this juncture we shall impose a restriction on the functions f_i whereby we shall only consider functions that are linear in x and that contain θ in a separable fashion; i.e. the performance equations shall be of the form shown in equation (C-3).

$$f_i = \sum_{i=1}^n a_{ij}\ x_j + \psi(\theta) \tag{C-21}$$

where a_{ij} is not necessarily constant.

For this class of functions we obviously have

$$\frac{\partial}{\partial x_j} f_i(\bar{x};\ \bar{\theta} + \delta\theta) = \frac{\partial}{\partial \bar{x}_j} f_i(\bar{x};\ \bar{\theta}) \tag{C-22}$$

and this fact causes the second integral in equation (C-20) to vanish; equation (C-20) then reduces to

$$\delta S = \int_0^T \sum_{i=1}^n z_i[f_i(\bar{x};\ \bar{\theta} + \delta\theta) - f\ (\bar{x};\ \bar{\theta})]dt$$

$$= \int_0^T [H(\bar{x};\ \bar{\theta} + \delta\theta) - H(\bar{x};\ \bar{\theta})]dt \tag{C-23}$$

Since S is to be maximized, it is necessary that δS be zero along the optimal trajectory for all free variations δθ and that δS be negative for variations δθ at the boundary of the constraints as expressed by equation (C-5). Therefore

$$\delta S \leq 0 \tag{C-24}$$

and hence by virtue of equation (C-23) it follows that

$$\delta H = H(\bar{x};\ \bar{\theta} + \delta\theta) - H(\bar{x};\ \bar{\theta}) \leq 0 \tag{C-25}$$

in the total interval

$$0 \leq t \leq T$$

Also, since equation (C-25) holds for any small perturbation $\delta\theta$, it is necessary for the Hamiltonian to take on a maximum value when S is to be maximized and on the other hand it is necessary for the Hamiltonian to be a minimum when S is to be minimized.

An interesting geometrical interpretation of the Maximum Principle may be obtained if one considers the fact that H is really the scalar product of the z(t) and f(x, θ) vector functions and that the θ(t) vector should be so mainpulated so as to maintain this scalar product at a maximum or minimum according as we wish to maximize or minimize the objective function.

C-2.2. FINAL TIME FIXED AND STATE VARIABLES WITH EQUALITY CONSTRAINTS

We shall now consider the case where the final state variables have equality constraints as follows,

$$F_\alpha[x(T)] = 0 \qquad \alpha = 1, 2, \ldots, p \quad p \leq n \tag{C-26}$$

Here we shall employ the variational technique using Lagrange Multipliers. Consider the objective function of the form

$$S = \sum_{i=1}^{n} C_i\ x_i(T) + \sum_{\alpha=1}^{p} \lambda_\alpha\ F_\alpha[x(T)] \tag{C-27}$$

instead of the original form

$$S = \sum_{i=1}^{n} C_i \; x_i(T)$$

and we desire to maximize S.

We see from equations (C-17) through (C-20) that

$$\sum_{i=1}^{n} z_i \delta x_i \Big|_0^T = \int_0^T \sum_{i=1}^{n} z_i [f_i(\bar{x};\ \bar{\theta} + \delta\theta) - f_i(\bar{x};\ \bar{\theta})]dt$$

$$+ \int_0^T \sum_{i=1}^{n} \sum_{j=1}^{n} z_i [\frac{\partial f_i(\bar{x};\bar{\theta}+\delta\theta)}{\partial x_j} - \frac{\partial f_i(\bar{x};\bar{\theta})}{\partial x_j} \quad \delta x_j]dt$$

(C-28)

In order that the left hand side of equation (C-28) represent the variation in the objective function, the boundary conditions of the z(t) vector have to be determined so that equation (C-25) holds.

From equation (C-27) we have

$$\delta S = \sum_{i=1}^{n} C_i \delta x_i(T) + \sum_{\alpha=1}^{p} \sum_{i=1}^{n} \lambda_\alpha \frac{\partial F_\alpha}{\partial x_i(T)} \delta x_i(T) + \text{higher order terms} \qquad \text{(C-29)}$$

If the constraints F_α have finite values for second order derivatives, then in the neighborhood of optimal values we may choose λ_α such that

$$\delta S = \sum_{i=1}^{n} [C_i + \sum_{\alpha=1}^{p} \lambda_\alpha \frac{\partial F_\alpha}{\partial x_i}] \; \delta x_i \Big|_{t = T} \qquad \text{(C-30)}$$

Now comparing the left hand side of equation (C-28) to equation (C-30), it is easy to see that

$$z_i(T) = [C_i + \sum_{\alpha=1}^{p} \lambda_\alpha \frac{\partial F_\alpha}{\partial x_i}]_{t=T} \qquad \text{(C-31)}$$

Therefore, we now have n equations from equation (C-1), n equations from equation (C-31) together with p equations from equation (C-26) with the help of which we can solve for the 2n unknown components of $x(t)$ and $z(t)$ and the p unknown components of λ_α. Equation (C-31) is equivalent to the transversality condition of the final values in the calculus of variations. A special case of the above problem is when only some of the final values of the state variable are fixed, say

$$x_i(T) = x_i^T \qquad i = 1, 2, \ldots, m$$

and the rest of the final values are still free. In this case, equation (C-20) becomes,

$$F_\alpha[x(T)] = x_i(T) - x_i^T = 0 \tag{C-32}$$

Substituting equation (C-32) into equation (C-31) yields

$$z_i(T) = [C_i + \lambda_i] \qquad i = 1, 2, \ldots, m \tag{C-33}$$

$$z_i(T) = C_i \qquad i = m+1, m+2, \ldots, n$$

Next let us consider the case where the constraints are imposed on the initial values of the state variables in the form

$$F_\beta[x(0)] = 0 \qquad \beta = 1, 2, \ldots, p \quad p \leq n \tag{C-34}$$

From equation (C-28) it follows that at the optimal condition

$$\sum_{i=1}^{n} z_i \, \delta x_i \Big|_{t=0}^{T} = 0 \tag{C-35}$$

If the initial values are preassigned, then $\delta x_i(0) = 0$ holds, and equation (C-18) is thereby satisfied. But if the initial values have a restriction as in the form of equation (C-34), then in general

$$\sum_{i=1}^{n} z_i \delta x_i \Big|_0^T = \sum_{i=1}^{n} C_i \delta x_i(T) - \sum_{i=1}^{n} z_i \delta x_i \Big|_{t=0}$$

$$- \delta S - \sum_{i=1}^{n} z_i \delta x_i \Big|_{t=0} = 0.$$

Since at the optimal condition we have $\delta S = 0$ it follows that

$$\Sigma z_i \delta x_i \Big|_{t=0} = 0 \qquad \text{(C-36)}$$

It should be noticed that the variation $\delta x_i(0)$ in equation (C-36) is under the restrictions of equation (C-34). Since small perturbations around optimal conditions have been considered, the variations $\delta x_i(0)$ lie on the planes tangent to the surfaces of equation (C-34). Equation (C-36) is the transversality condition of the initial values.

C-2.3. FINAL TIME UNSPECIFIED

The previous cases considered were characterized by a fixed final time T, we shall now consider the case where the final time T is free and is to be determined along with the optimal state vector $\overline{x}(t)$ and the optimal decision vector $\overline{\theta}(t)$. This is what is known as the time optimal problem.

If the final time T appears in the objective function, we introduce an n+1 state variable x_{n+1} such that

$$\frac{dx_{n+1}}{dt} = 1, \qquad x_{n+1}(0) = 0 \tag{C-37}$$

and $x_{n+1}(T)$ is identical to T itself.

$$\delta S = \sum_{i=1}^{n+1} \frac{\partial S}{\partial x_i(T)} \delta x_i(T)$$

$$= \sum_{i=1}^{n+1} \frac{\partial S}{\partial x_i} \frac{dx_i}{dt} \delta t \Big|_T$$

Then it follows from the above equation and equation (C-30) that

$$\delta S = \sum_{i=1}^{n+1} \left[C_i + \sum_{\alpha=1}^{p} \lambda_\alpha \frac{\partial F_\alpha}{\partial x_i(T)} \right] \frac{dx_i}{dt} \delta t \Big|_{t=T}$$

$$= \sum_{i=1}^{n+1} z_i \frac{dx_i}{dt} \delta t \Big|_{t+T} \tag{C-38}$$

Since we want to maximize S, $\delta S \leq 0$. But on the other hand δt may take positive or negative values and therefore as S attains its maximum value δS must equal zero. It therefore, follows that

$$H(T) = \sum_{i=1}^{n+1} z_i \frac{dx_i}{dt} \Big|_{t+T} = 0 \tag{C-39}$$

Also since H has a constant value throughout the transient state, it follows that

$$H = 0, \qquad 0 \leq t \leq T$$

is a necessary condition for optimality when the final time T is unspecified.

2.4 EXISTENCE THEOREMS OF MARKUS AND LEE [13]

Theorem 1. Given the control problem

(a) $\dot{x}_i = f_i(t, x_1, x_2, \ldots, x_n, u_1, \ldots, u_m)$

$$= g_i(t, x) + h_i^j(t, x)\, u_j \qquad i = 1, 2, \ldots, n$$

$$j = 1, 2, \ldots, m$$

with

$$g_i(t, x),\ h_i^j(t, x),\ \frac{\partial g_i(t, x)}{\partial x_k},\ \frac{\partial h_i^j(t, x)}{\partial x_k}, \quad k = 1, 2, \ldots, n$$

continuous in all their variables,

(b) a nonempty, convex, compact restraint set Ω in R^m,

(c) the initial point x_o in R^n,

(d) the continuously moving nonempty compact target set $G(t)$ on a finite interval $\gamma_o \leq t \leq \gamma_1$,

(e) the cost functional

$$C(u) = \int_{t_o}^{t_1} f_o(t, x(t), u(t))dt$$

where $f_o(t, x, u) = g_o(t, x) + h_o^j(t, x)u_j$ and the functions $g_o(t, x)$ and $h_o^j(t, x)$, $j = 1, 2, \ldots, m$ are continuous in all their variables.

Assume the set Δ of controls with responses traveling from x_o to G is such that

(A) Δ is non empty

(B) there exists a real bound $B < \infty$ for all responses $x(t)$ corresponding to $u(t)$ in Δ, that is, $|x(t)| = \sum_{i=1}^{n} |x_i(t)| < B$ uniformly for all responses.

Then there exists an optimal control $u^*(t)$ in Δ.

Remark: Hypothesis B of theorem 1 is satisfied for x in R^n and u in Ω if

$$\left| f_i(t, x, u) \right| < \alpha, \qquad i = 1, 2, \ldots, n$$

or if

$$\left| \frac{\partial f_i(t, x, u)}{\partial x_j} \right| < \alpha, \quad i = 1, 2, \ldots, n$$

for some real α. Hypothesis A of theorem 1 deals with the question of whether or not the system can be moved from x_o to G(t) in a finite time. The set of initial points C_o from which the system can be moved to G(t) in a finite time is called the domain of controllability and is the subject of the next theorem.

Theorem 2. Consider

$$\frac{dx_i}{dt} = f_i(x_1, \ldots, x_n, u_1, \ldots, u_m), \qquad i = 1, \ldots, n$$

where f(x, u) and $\frac{\partial f}{\partial u}(x, U)$, and $\frac{\partial f}{\partial x}(x, u)$ are continuous in $R^n \times \Omega$. The control restraint $\Omega \subset R^m$ contains the origin in its interior.

Assume:

(1) $f(0, 0) = 0$

(2) There exists a vector $v \in R^m$ such that $Bv, ABv, \ldots, A^{n-1}Bv$, are linearly independent, where $A = \frac{\partial f_i}{\partial x_j}(0, 0)$ and $B = \frac{\partial f_i}{\partial u_k}(0, 0)$, $i = 1, 2, \ldots, n$; $k = 1, 2, \ldots, m$.

Then there exists a neighborhood $U \in R^n$ of the origin such that each point $x_o \in U$ can be steered to the origin in R^n in a finite time interval, using a measurable control function $u(t)$ with graph in Ω. Remark: Hypothesis (2) is satisfied if

$$\det [Bv, ABv, \ldots, A^{n-1} Bv] \neq 0.$$

EFFECTS OF LIQUID PHASE MIXING ON CONTROL OF
A DISTILLATION COLUMN

by

NORMAN C. PEREIRA

B. Sc. (Chemistry), Bombay University, India 1963

B. S. (Ch. Eng.), Tulsa University, Oklahoma 1966

AN ABSTRACT OF A MASTER'S THESIS

submitted in partial fultillment of the

requiremtents for the degree

MASTER OF SCIENCE

Department of Chemical Engineering

KANSAS STATE UNIVERSITY
Manhattan, Kansas

1969

ABSTRACT

Most of the literature dealing with control of distillation columns considers simplified models of complete mixing to represent the liquid phase mixing on the distillation trays. In this work a two tray distillation column is considered wherein the top tray is described by the so-called mixing pool model consisting of two tanks in series. Also for the sake of comparison a conventional distillation column with complete mixing on the top tray is also considered. The control problem is defined thus: the system suffers a disturbance through the feed composition which in turn displaces the overhead distillate composition from its steady value. Determine a control policy for the overhead reflux rate such that a) the overhead distillate composition will be returned to its steady state value in the shortest possible time b) the overhead distillate composition will be returned to its steady state value and in doing so its deviation from the steady state value will be minimum in a least squares sense. Both problems a) and b) are applied to both systems described above and their corresponding control policies are obtained. It is found that the change in the model has a significant effect on the control policy and on the methods of obtaining the control policies. Various extensions to the present problem are also suggested.