

DEVELOPMENT OF FEED CHANGEOVER POLICIES
FOR REFINERY DISTILLATION UNITS

by

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ERRATA

- p. 7 2nd line from bottom: CONCULSIONS should be CONCLUSIONS
- p. 15 Eqn. 2.6 J_u^T : transpose missing
- p. 16 Eqn. 2.9 J_u^T : transpose missing
- p. 18 10th line from bottom: developemnt should be development
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ABSTRACT

This work is concerned with a two-stage approach to the synthesis of feed changeover policies for refinery distillation units. Firstly, off-line open-loop optimal control studies are performed. Sub-optimal control laws are then proposed which retain the dominant features of the optimal responses yet allow for the practical aspects of implementation.

A numerically efficient optimal control package was established for non-linear systems described by ordinary differential equations. The algorithm is in the form of a non-linear program with piecewise constant control levels and switching times as the decision variables. It is capable of solving problems with stiff differential equations, fixed or free end times, bounds on the control variables, as well as final time and path constraints on functions of the states and controls. Owing to structural similarities of the state and adjoint differential equations, it was found that implicit linear multi-step integration procedures exhibited computational savings over standard explicit methods, even for non-stiff systems. The effectiveness of the package is demonstrated by chemical engineering examples.

The feed changeover problem, for movement of operation between two optimal steady states, was then formulated as an optimal control problem. A method was developed that ensured equivalence of optimal steady state profit conditions between dynamic models adopted for control purposes and simpler steady state models used in the context of overall refinery optimization. Preliminary calculations showed that maximization of profit yielded similar control trajectories to minimization of off-specification product.

The optimal ordering of the product stream specification changeovers was determined by simple a priori policies.

Optimal control calculations were performed to minimize off-specification product for three refinery distillation units of varying complexity. Fast feed changeovers were found to be effected by the entire contents of the column becoming either heavier or lighter together. Implementable sub-optimal policies based upon this observation take the form of feedforward control levels with switching between these levels governed by simple feedback laws. Simulation of these policies revealed close agreement with the optimal responses.

TO MY MOTHER

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CHAPTER 1 - INTRODUCTION

In recent years, the strained economic and political climate associated with the production of crude oil has resulted in a large increase in the price of refinery feedstocks. Oil companies cannot fulfill their market demand with crude from a single source and therefore are forced to rely on a variety of crude reserves. Consequently, some refineries will undergo crude changes which invariably mean off-specification products. As feed costs increase, changeover operating policies become more important and with oil reserves predicted to dwindle in the future, the problem can only be expected to magnify.

In order to develop suitable changeover control policies for a particular refinery, a joint project was recently established between BP and the Chemical Engineering Department of Imperial College of Science and Technology. The current operating practice for crude changes at this refinery relies heavily on operator experience. From a production planning linear program, the operator has a list of product specifications and control settings for each crude which represents the steady state optimum. Since no changeover policies exist, the control of the dynamic period is governed solely by the operator. Naturally, controls are not consistent and may alter drastically, even from shift to shift.

Most control system synthesis in the refinery field is based on dynamic models which relate the responses of state variables (i.e. qualities and flowrates) to control variables (i.e. reflux rates, product takeoffs, heating rates) and to load

disturbances (i.e. feed temperature, composition, and flowrate). As a result of on-site identification experiments, BP have recently furnished dynamic models of three distillation units: a debutanizer, a splitter, and an atmospheric crude unit. Together, these units provide the feedstock for the entire refinery operation. Since good control of these columns implies less prolonged disturbances for downstream units, work at this stage is confined to the three specified units.

There are many available methods for performing the control system design, but before one is chosen the nature of the processes and disturbances should be considered. The BP models are represented by non-linear differential equations and the upsets for typical crude changes are known to be large. Therefore, the use of any design method based on linear theory, without successive linearization, can be dismissed. Because the time at which the upsets occur are known, some anticipatory action before the disturbances enter a unit could be useful. Thus, any feedback design method, unless coupled with feedforward elements, would not be adequate.

Most methods allow the design of suitable controllers for a specified control structure. However, the more fundamental problem is to determine the control structure that will result in good system performance. Some advances in this direction have recently occurred in linear feedback control. Rosenbrock's (1974) inverse Nyquist multivariable design procedure has proved successful in several industrial applications. Non-interacting design has been proposed as an analytical tool for the pairing of control and measurement variables in binary distillation columns (Shinskey, 1967). Because both these methods establish

the feedback configuration based upon a local linearization of a steady state, the structures would be expected to alter for large changes in the operating conditions. Far more latitude, in terms of control system synthesis, can be derived from the optimal control design technique. For the open loop structure, the time varying controls are calculated in order to minimize an objective function representative of system performance. In this manner, interactions and non-linearities are dealt with naturally. Any special feedforward or feedback structure could be deduced from the optimal response curves.

Recently, the optimal control philosophy has been at the centre of some controversy. In 1973, optimal control was heavily criticized (Foss, 1973) with complaints of difficult and lengthy computations. Foss also indicated that startups, shutdowns, and changeovers occur too infrequently for optimal control to be useful and that the results are presented in open loop rather than feedback form. Kestenbaum et al. (1976) have compared a classical PID controller with optimal feedback controllers and found that the PID action out-performed the optimal controller on the basis of six design criteria. It is interesting to note that only the feedback, and not the feed-forward, nature of the optimal controllers were tested. The use of off-line optimal control for designing on-line feedback controllers from open-loop responses has been defended by Sargent (1975) with reference to a successful application in a tubular chemical reactor (Joffe and Sargent, 1972). Other areas of optimal control applications for control system synthesis include steel rolling mills (Bryant, 1975) and catalytic crackers (Kurihara, 1967). The particular problem of interest

here is that of a changeover and feedforward action is expected to be implemented. Since an off-line method is required to develop a control system structure, optimal control appears to be the ideal tool.

The optimal control problem is formulated as a set of state and adjoint differential equations with two-point boundary conditions. The problem can be solved by several methods such as dynamic programming and direct solution of the two-point boundary value problem. For chemical engineering systems, control vector iteration is accepted as the best available procedure (Lapidus and Luss, 1967). Once the continuous control trajectories are discretized (e.g. piecewise constant, piecewise linear), the optimal control problem is reduced to a nonlinear programming problem in which the discretized controls and possibly switching times are selected in order to minimize an objective function. Convergence of optimal control problems solved in this manner has been found to be sensitive to the choice of the method which drives the controls and switching times to their optimal values (Pollard and Sargent, 1970b; Rao and Luus, 1972). The evaluation of the objective function requires integration of the state differential equations, and for distillation systems these are usually stiff (Mah et al., 1962; Tyreus et al. 1975). This means that the eigenvalues of the Jacobian of the right hand side of the differential equations are widely spread which results in a very slow integration if standard routines (e.g. Runge-Kutta) are used. In Chapter 2, the structure of the optimal control problem is examined and a computationally efficient optimal control algorithm is developed and tested.

Chapter 3 is concerned with the formulation of crude changeovers as optimal control problems. The suitability of various dynamic distillation models, including the supplied BP models, is considered. A large sophisticated model which exactly represents the dynamics of the system would be computationally cumbersome but a smaller inaccurate model would produce off-line responses that could not be duplicated on the plant. The compromise between model order and calculational ease is referred to as the principle of optimum sloppiness (Lee and Weekman, 1976). The sensitivity of the optimal controls to the choice of objective function is also examined. Total profit throughout the changeover period may be the realistic measure of performance but this could be difficult to estimate for an isolated unit, particularly if the products are blended after several units downstream. Alternatively, minimum time to reach the new steady state or the familiar squared deviation from set point are objective function candidates.

In principle, the optimal control algorithm which is developed here could determine the optimal control of the three column integrated system, but this would be a formidable task, even with today's large scale computers. For the purposes of this exercise, the three columns are studied separately and three control systems are designed separately. There are several other justifications for this. One is the fact that the identification experiments were proceeding at the same time as this work and the optimal control calculations were performed as the models became available. Another is the implementation aspect. If the results led to a three column integrated control system, the construction proposal would either be accepted or rejected on

economic grounds without experimental support. However, if control system designs were presented for three separate columns of varying complexity, the smallest system could be implemented at relatively little expense and if successful, it would provide an incentive for the larger investment.

Several methods exist for performing the control system synthesis using the off-line optimal results. If a control function structure is assumed (e.g. polynomial), the control at any moment in time could be statistically correlated to the current or recent measurable state (Bhandari, 1970) and possibly future upsets to give a feedback control law. However, the large, time-varying correlation matrix would probably exhibit high model sensitivity and it would be necessary to retune it on-line. Perhaps a better approach would be to identify important interactions and unifying features of the responses and then to exploit these in the control system design (Joffe and Sargent, 1972). A control structure is then determined that allows the important trajectories to approximate those of the optimal responses, by use of simple control laws. Although off-line guidelines could be established, these control laws would be tuned on-line. Furthermore, the improved physical understanding of the process that is gained by such an analysis would be useful for future control studies. The optimal control and control system synthesis for the three units are undertaken in Chapter 4 and Chapter 5.

CHAPTER 2 - DEVELOPMENT OF AN EFFICIENT OPTIMAL

CONTROL PACKAGE

2.1 Problem Formulation and Previous Work

2.1.1 Statement of the Optimal Control Problem

Consider the system governed by the set of differential equations:

$$\dot{x} = f(x, u, t) ; x(0) \text{ given} \quad (2.1)$$

where:

x is an n dimensional state vector,

u is an nc dimensional control vector,

f is an n dimensional vector function,

t is time.

The performance of the system is measured by a scalar objective function given by:

$$I = \phi(x(t_f), t_f) + \int_0^{t_f} J(x, u, t) dt \quad (2.2)$$

where:

t_f is the final time of operation

The system may be subject to several types of constraints of the form:

$$u_{\min} \leq u \leq u_{\max} \quad (2.3)$$

$$g_{\min} \leq g(x(t_f), t_f) \leq g_{\max} \quad (2.4)$$

$$a_{\min} \leq a(x, u, t) \leq a_{\max}, \quad t \in [0, t_f] \quad (2.5)$$

where g and a are vectors of dimension p and q respectively.

Eq. (2.3) represents any plant limitations such as maximum flow-rates or heat inputs. Sometimes it becomes necessary to specify bounds for final product qualities or ensure that a unit is in a

reasonable state at the final time to continue operation; in these situations constraints of the type given by Eq.(2.4) must be considered. Path constraints, which are denoted by Eq.(2.5) guarantee that conditions do not arise at any time which would lead to an unfavourable occurrence such as catalyst contamination or off-specification product. The optimal control problem is then to choose the time varying controls, $u(t)$, to minimize the performance index (2.2) subject to Eq.(2.1), (2.3), (2.4) and (2.5). In the free end time problem, the final time, t_f , must be selected in addition to the controls in order to minimize I .

2.1.2 Methods for the Solution of Optimal Control Problems

The solution to the optimal control problem outlined in the previous section has been an area of active research interest for the past fifteen years. Firstly, consider only the unconstrained problem of minimizing the performance index given by Eq.(2.2) subject to Eq.(2.1). The development of the necessary conditions for the solution to this problem using the calculus of variations is well known (Bryson and Ho, 1969). At the optimum, the following equations hold:

$$f_u^T \lambda + J_u = 0 \quad t_0 \leq t \leq t_f \quad (2.6)$$

where the n -dimensional adjoint vector, λ , is specified by:

$$\dot{\lambda} = -f_x^T \lambda - J_x^T \quad (2.7)$$

$$\lambda(t_f) = \phi_x^T \quad (2.8)$$

Eq.(2.1), (2.6), (2.7) and (2.8) represent a two-point boundary value problem (TPBVP) whose solution yields the optimal control. Although many methods exist for solving the TPBVP, it is generally

accepted that for high order systems, as characterized by chemical engineering multistage operations, control iterative procedures provide the best approach (Lapidus and Luus, 1967; Bryson and Ho, 1969). These algorithms successively update the control to improve the objective function while constantly satisfying the boundary conditions given by Eq.(2.1) and (2.8).

In order to transform the problem into an unconstrained optimization exercise, the control is usually assumed to be piecewise constant over an integration interval. Earlier methods relied on steepest descent to drive the controls and thus required gradients of the objective function with respect to the controls. At any point in time, these are given by:

$$I_u = f_u^T \lambda + J_u \quad (2.9)$$

Convergence properties of steepest descent were found to be slow, especially near the optimum. Second variation methods overcame this problem, but at the expense of increased storage and more coding effort. Lasdon et al. (1967) presented the conjugate gradient method (Fletcher and Reeves, 1964) as a compromise with slightly slower convergence but with increased simplicity over second variation algorithms. Tokumaru et al.(1970) proposed the variable metric approach of Davidon (1959). This method belongs to the general class of quasi-Newton procedures which exhibit faster convergence than conjugate gradient algorithms, but require more storage. Rao and Luus (1972) compared 17 versions of steepest descent, second variation, conjugate gradients and quasi-Newton methods on four chemical engineering optimal control examples. Their results confirm the observations stated above

and are consistent with the findings of Sargent and Sebastian (1972) for unconstrained optimization methods.

For optimal control problems where constraints given by Eq.(2.3), (2.4) and (2.5) occur, the situation is not as tidy. Penalty function methods that simply add constraint violations to the objective function usually spend more time satisfying the constraints than optimizing the performance index. Final time constraints will normally be non-linear with respect to the control because of the influence of the state through the system equations. Some authors (Miele et al., 1970; Heidman and Levy, 1975) have treated optimal control problems with final time constraints with a sequential-gradient-restoration algorithm. After each step in the gradient method the restoration algorithm regained feasibility by minimizing the squared change in the control. In reality, this is a simple non-linear program using an unconstrained method as a driving routine. Rosen (1966) implemented a non-linear programming approach to solve linear discretized problems with bounded controls, path and final time constraints. The same technique is utilized by Ho and Brentani (1963) to deal with the non-linear system equations with only inequality constraints on the control.

The application of non-linear programming to the optimal control problem would necessitate gradients of the constraints with respect to the control. If the previously mentioned unconstrained algorithms were extended to encompass non-linear constraints, the storage demand on even large computers are dramatic and therefore simplifications are sought. Recently, Nishida et al. (1976) applied the Max-H algorithm, which treats bounds on the control, to several chemical engineering problems.

Theoretically, the method can only deal with bang-bang control policies but a penalty function limiting process with an integral quadratic control term provides approximations to singular policies. Although the Max-H algorithm is capable of determining sub-optimal trajectories for bounded controls, the extension to include final time and path constraints does not appear obvious.

Rather than approximate the solution as the Max-H strategy does, if the problem could be simplified, then efficient numerical methods could possibly still be used. Some investigators have employed piecewise constant (Horwitz and Sarachik, 1968; Pollard and Sargent, 1970 a,b) or piecewise linear controls (Joffe and Sargent, 1972) over more than one integration step for the unconstrained problem. Thus, the control space is reduced, sometimes drastically. In many cases, where system models are not accurate, or where measurements are not precise, such a simplification is justified. It is certainly appropriate for the approach adopted here in which the off-line optimal responses are used as guidelines in the development of on-line control policies. However, the problem still remains of establishing an algorithm in the context of non-linear programming that can effectively handle all types of constraints. Such an algorithm is presented in the following sections.

2.2 Application of Non-linear Programming to Optimal Control Problems

In this section, the formulation of the non-linear program that solves optimal control problems with piecewise constant bounded controls, final time and path constraints will be

considered. No attempt will be made in this work to discriminate between various non-linear programming algorithms. Instead, one proven method, variable metric projection (VMP) (Sargent and Murtagh, 1973; Sargent and Gaminibandara, 1975), will provide a basis for the development of numerical procedures. However, the application of other non-linear programs would be simple since any efficient algorithm requires the same user supplied input information as VMP. Before the optimal control problem is formulated, this information should be examined.

2.2.1 Non-linear Programming

Non-linear programs attempt to minimize the objective function subject to linear and non-linear constraints. In mathematical terms, the problem can be expressed as follows:

Choose: y

To minimize: $I(y)$

- Subject to: $y_{\min} \leq y \leq y_{\max}$ (2.10)

$l_{\min} \leq l(y) \leq l_{\max}$ (2.11)

$nl_{\min} \leq nl(y) \leq nl_{\max}$ (2.12)

where y is an r dimensional vector of optimization variables,

l is an s dimensional vector function of linear constraints,

and nl is a v dimensional vector function of non-linear

constraints. Basically, VMP uses a variable metric to

account for quadratic approximations to objective and non-linear constraint functions, and updates y in constraint space.

Although the linear constraints are always satisfied, each step usually moves into the infeasible region along the tangent

hyperplane of the non-linear constraints. At this point a Newton correction procedure is applied to reestablish feasibility. By using the correction algorithm in an initial phase to minimize the constraint violations, a non-feasible starting point is permitted. VMP has been shown to be successful on standard non-linear test problems (Sargent and Murtagh, 1973) as well as on steady state distillation optimization (Sargent and Gaminibandara, 1975). Furthermore, in considering possible optimization methods for constrained optimal control, Wierzbicki (1974) highly recommends projected gradient methods.

Apart from the obvious input requirements such as starting point, constraint bounds, and stopping tolerance the following information must be supplied:

- (a) the initial values of the linear constraints, $l(y)$
- (b) l_y , matrix of gradients of linear constraints with respect to y
- (c) a subroutine to evaluate $I(y)$ given y
- (d) a subroutine to evaluate $nl(y)$ given y
- (e) a subroutine to evaluate vector I_y , gradients of the objective function with respect to y , given y
- (f) a subroutine to evaluate matrix nl_y , gradients of non-linear constraints with respect to y , given y .

The theory upon which non-linear programming is established demands that objective and non-linear functions and gradients are continuous.

2.2.2 Formulation of the Optimal Control Problem

The optimal control problem stated in section 2.1 can now be formulated in terms of the non-linear programming structure

shown in section 2.2. The optimization variables are chosen to be piecewise constant control levels and switching times. For the free end time problem the final time is considered to be an additional switching time. If the time period is discretized into NCI control intervals, the optimization variable vector y becomes:

$$y = [u^1, t^1, u^2, t^2, \dots, u^i, t^i, \dots, t^{NCI-1}, u^{NCI}, t_f]^T \quad (2.13)$$

where u^i is the nc -dimensional piecewise constant control vector in the i th interval,
 t^i is the time at which the control interval index changes from i to $i + 1$.

Thus, y has dimension $(nc + 1)NCI$. The time varying control trajectory, $u(t)$, is then given by:

$$u(t) = u^1 \quad ; \quad 0 \leq t < t^1 \quad (2.14)$$

$$u(t) = u^i \quad ; \quad t^{i-1} \leq t < t^i, \quad i = 2, 3, \dots, NCI-1 \quad (2.15)$$

$$u(t) = u^{NCI} \quad ; \quad t^{NCI-1} \leq t \leq t_f \quad (2.16)$$

In principle, a switching time vector could have been formed consisting of a switch time for each element of the control vector in each control interval. However, since storage requirements in VMP are approximately proportional to the square of the number of optimization variables, the single switch simplification results in almost four-fold storage reduction for cases where nc is large. Similarly, the same compromise between storage and accuracy can be achieved by altering the number of control intervals. As NCI approaches the number of integration steps,

the control trajectory becomes continuous but at the expense of increased core memory.

There are several approaches available to derive the necessary gradients. For the unconstrained case, Bryson and Ho (1969) use the adjoint vector, λ , to "adjoin" the system equations in form of constraints to the objective function. The adjoint equation and its boundary condition appear following some mathematical manipulations after which variational methods are applied to obtain the gradients. Other authors (Polak (1971); Sargent and Sullivan (1977)) have assumed a more direct approach. By treating the problem as one of optimization, they introduced an adjoint system that allowed the evaluation of gradients for any final state function of the states. Since this method effects a simple, straightforward extension to the non-linear constraint case, it will be adopted here.

A new state variable is added to account for integral terms in the objective function. Define:

$$\dot{x}_{n+1} = J(x,u,t) \quad ; \quad x_{n+1}(0) = 0 \quad (2.17)$$

Eq.(2.2) can now be expressed in the form:

$$I = F(x(t_f)) \quad (2.18)$$

The minimum time problem is formulated by defining:

$$\dot{x}_{n+1} = 1 \quad (2.19)$$

$$F = x_{n+1} \quad (2.20)$$

where n is the dimension of the state including the previous augmentation. The gradients of the objective function with respect to the optimization variables are then given by (Pollard and Sargent, 1970b):

$$\frac{\partial F}{\partial u^i} = \int_{t^{i-1}}^{t^i} \lambda^T f_u dt ; \quad i = 1, 2, \dots, NCI \quad (2.21)$$

$$\frac{\partial F}{\partial t^i} = \lambda^T(t^i) [f(x(t^i), u^i, t^i) - f(x(t^i), u^{i+1}, t^i)]$$

$$i = 1, 2, \dots, NCI-1 \quad (2.22)$$

where the adjoint vector, λ , is given by:

$$\dot{\lambda} = -f_x^T \lambda ; \quad \lambda(t_f) = F_x^T \quad (2.23)$$

For the free end time problem, the relevant gradient is:

$$\frac{\partial F}{\partial t_f} = \lambda^T(t_f) \cdot f(x(t_f), u(t_f), t_f) \quad (2.24)$$

The objective function and gradients are obtained by integrating Eq.(2.1) forward, evaluating $F(x(t_f))$ and $F_x(x(t_f))$, integrating Eq.(2.23) backwards, and simultaneously calculating derivatives using Eq.(2.21), (2.22), and (2.24).

Now consider end time constraints as given by Eq.(2.4).

Since these are simply final time functions, there is no reason why a similar adjoint system cannot be employed. Define:

$$\dot{\lambda}_1 = -f_x^T \lambda_1 ; \quad \lambda_1(t_f) = g_x^T \quad (2.25)$$

where λ_1 is an $n \times p$ matrix of adjoints. The gradients are derived in the same manner as for the objective function with the addition of terms to account for the direct influence of the final control levels and end times on the constraints.

This yields the following derivative expressions:

$$\frac{\partial g}{\partial u^i} = \int_{t^{i-1}}^{t^i} \lambda_1^T f_u dt \quad ; \quad i = 1, 2, \dots, NCI-1 \quad (2.26)$$

$$\frac{\partial g}{\partial u^{NCI}} = \left. \frac{\partial g}{\partial u} \right|_{t=t_f} + \int_{t^{NCI-1}}^{t_f} \lambda_1^T f_u dt \quad (2.27)$$

$$\frac{\partial g}{\partial t^i} = \lambda_1^T(t^i) [f(x(t^i), u^i, t^i) - f(x(t^i), u^{i+1}, t^i)]$$

$$i = 1, 2, \dots, NCI-1 \quad (2.28)$$

$$\frac{\partial g}{\partial t_f} = \left. \frac{\partial g}{\partial t} \right|_{t=t_f} + \lambda_1^T f(x(t_f), u(t_f), t_f) \quad (2.29)$$

The procedure for calculating non-linear constraint functions and gradients is exactly the same as that outlined for the objective function.

Path constraints, as represented by Eq.(2.5), have always been the stumbling block for optimal control problems. The time varying nature could be overcome by discretization, but this would add numerous non-linear constraints to an already large problem. Some investigators (Bryson and Ho, 1969; Lapidus and Luus, 1967) have suggested to augment the performance index with the integrated constraint function violations. Rather than resort to penalty functions, a better approach would be to constrain the integrated violations to zero at the final time. In this manner, the previously developed theory for final time constraints could be utilized. Define a new state variable as:

$$\begin{aligned}\dot{x}_{n+1} &= (a_{\min} - a)^T W_1 (a_{\min} - a) + (a - a_{\max})^T W_2 (a - a_{\max}); \\ x_{n+1}(0) &= 0\end{aligned}\quad (2.30)$$

where n is the augmented state dimension,

W_1 and W_2 are $q \times q$ diagonal weighting matrices whose elements reflect feasibility with respect to the path constraint. That is:

$$W_{1jj} = 0 \quad ; \quad a_j - a_{j_{\min}} > 0 \quad ; \quad j = 1, 2, \dots, q \quad (2.31)$$

$$W_{1jj} = 1 \quad ; \quad a_j - a_{j_{\min}} \leq 0 \quad ; \quad j = 1, 2, \dots, q \quad (2.32)$$

$$W_{2jj} = 0 \quad ; \quad a_{j_{\max}} - a_j > 0 \quad ; \quad j = 1, 2, \dots, q \quad (2.33)$$

$$W_{2jj} = 1 \quad ; \quad a_{j_{\max}} - a_j \leq 0 \quad ; \quad j = 1, 2, \dots, q \quad (2.34)$$

Construct a new final time constraint:

$$x_{n+1}(t_f) = 0 \quad (2.35)$$

It is clear that when constraint (2.35) is satisfied, the state and control trajectories are feasible with respect to the path constraints. The gradients of the right hand side of Eq.(2.30) are continuous with state and controls, and therefore the continuity of final state constraint function and gradients is ensured.

The gradient of the right hand side of Eq.(2.30) with respect to the control, u , is given by:

$$f_{n+1u} = -2(a_{\min} - a)^T W_1 a_u + 2(a - a_{\max})^T W_2 a_u \quad (2.36)$$

Note that when constraint (2.35) is satisfied, the gradient, f_{n+1u} , has the value zero. Upon substitution into Eq.(2.26), this results in a zero gradient of the constraint (2.35) with respect to the control over the entire time period. In the non-linear program then, any projection will not account for the presence

of the non-linear path constraints, and hence will rely on the restoration algorithm to regain feasibility after an unconstrained step has been taken. Strictly speaking, with zero constraint gradients at the optimum, the constraint optimality conditions are not valid. However, since non-linear projection methods explore spaces within a tolerance of the constraint bounds where these gradients are non-zero, convergence can be assured. For equality constraints, where $a_{\min} = a_{\max}$, zero gradients only occur on the constraint, and for the reasons stated above, this type of constraints should present no problem.

In order to guarantee that constraint optimality conditions hold at the solution, consider, instead of Eq.(2.30), the following equation:

$$\dot{x}_{n+1} = e_1^T(a_{\min} - a) + e_2^T(a - a_{\max}) \quad ; \quad x_{n+1}(0) = 0 \quad (2.37)$$

where e_1 and e_2 are column vectors of dimension q whose elements are chosen in the same manner as elements of W_1 and W_2 respectively according to Eq.(2.31) - (2.34). The gradient, f_{n+1_u} , is then given by:

$$f_{n+1_u} = (e_1^T - e_2^T)a_u \quad (2.38)$$

When constraint (2.35) is not satisfied:

$$f_{n+1_u} = \pm a_u \quad (2.39)$$

and the gradient given by Eq.(2.26) is generally non-zero. However this approach has some drawbacks. Within the feasible region the constraint gradient is zero, but at the bound it jumps to a value given by Eq.(2.38). This discontinuous nature of the gradient

is contradictory to the assumptions used in proving convergence for projection methods, although this may not have a significant effect. If a step is taken from an interior point and a constraint is encountered, it will simply be added to the active set and progress will be made along that constraint, for which the gradient is defined. Secondly, the gradient jump may result in a non-unique adjoint integration in that a branch point could occur at the jump. For these reasons, the form of Eq.(2.30) will be assumed.

In order to demonstrate some of these ideas concerning path constraints, consider the following very simple example:

Choose: $u(t)$

To minimize: $\int_0^1 x_1 dt$

Subject to: $\dot{x}_1 = u$; $x_1(0) = 0$ (2.40)

$x_1(t) > 0$; $t \in [0,1]$ (2.41)

The solution to this problem is clearly:

$u(t) = 0$; $t \in [0,1]$ (2.42)

In terms of the structure presented previously, the problem would be reformulated as:

Choose: $u(t)$

To minimize: $I = x_0(1)$ (2.43)

Subject to: $\dot{x}_0 = x_1$; $x_0(0) = 0$ (2.44)

$\dot{x}_1 = u$; $x_1(0) = 0$ (2.40)

$\dot{x}_2 = \{\min[0, x_1]\}^2$; $x_2(0) = 0$ (2.45)

$g = x_2(1) = 0$ (2.46)

For simplicity, choose NCI equal to unity (i.e., the control, u , remains constant over the entire period of operation). With this structure it can easily be shown that the objective and constraint functions are given by:

$$I = u/2 \quad (2.47)$$

$$g = u^2/3, \quad u < 0 \quad (2.48)$$

$$g = 0, \quad u \geq 0 \quad (2.49)$$

A plot of the objective and constraint functions versus the control is shown in Fig. 2.1. It is clear that minimization of the objective subject to constraint feasibility is achieved at $u = 0$. The reduced form of the problem given by Eq.(2.47) - (2.49) was solved using the constrained optimization method (VMP) of Sargent and Murtagh (1973). A tolerance on the constraint function was set at 10^{-5} (i.e. $-10^{-5} < g < 10^{-5}$). In order to circumvent problems associated with zero constraint gradients for positive values of u , Eq.(2.49) was replaced by:

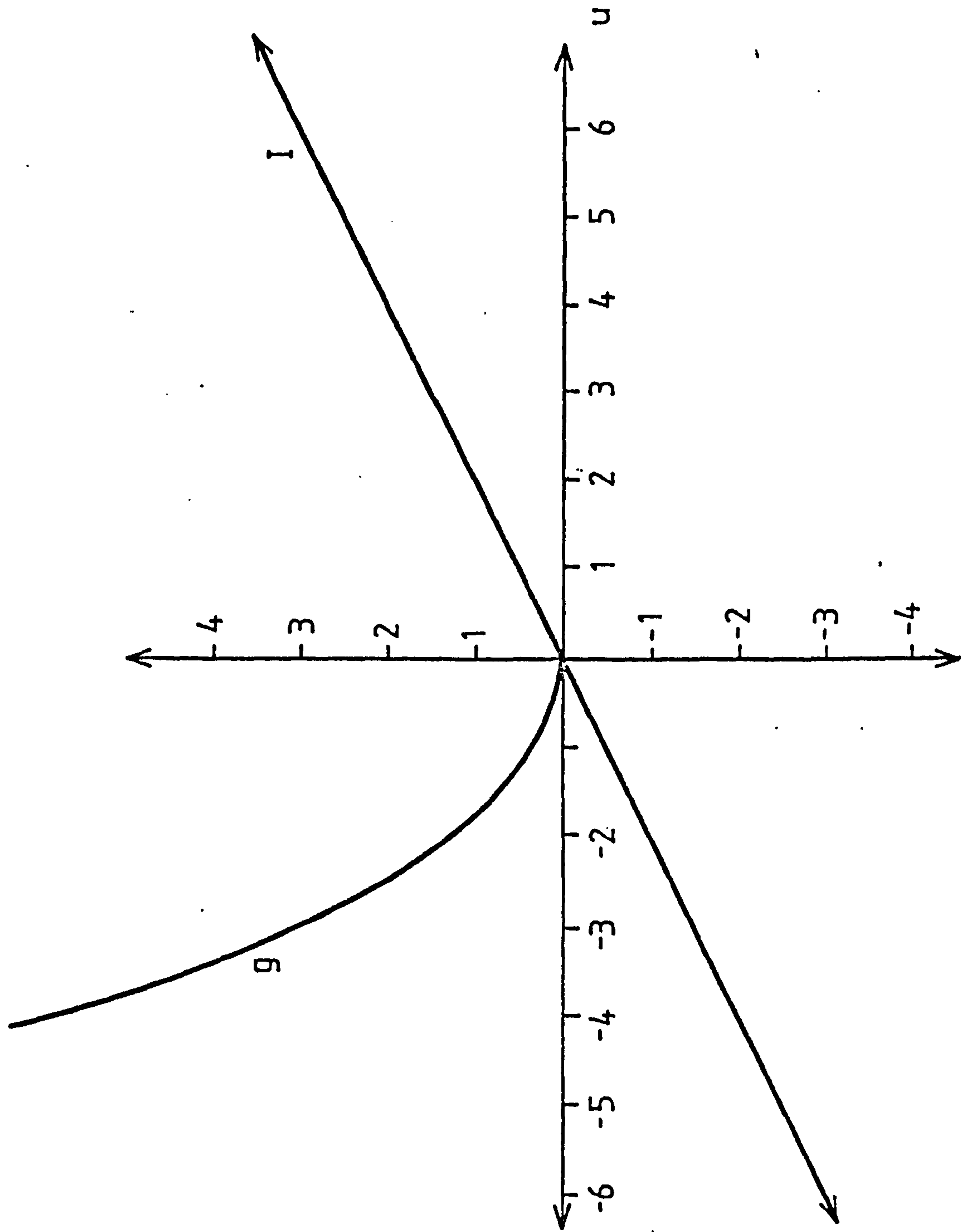
$$g = 10^{-8}u, \quad u \geq 0 \quad (2.50)$$

Thus, the constraint is satisfied and has a positive gradient for $u < 10^3$, which is unlikely to be violated for any reasonable starting point. VMP converged to the solution ($u = 7.5 \times 10^{-27}$) in two steps from a starting point of $u = 5$. This demonstrates that the proposed algorithm is capable of dealing with path constraints.

The non-linear program which represents the optimal control problem can now be formulated. It is assumed the all path constraints are expressed by a single final time constraint which is lumped into Eq.(2.4). The general non-linear programming formulation, as outlined in Eq.(2.10) - (2.12) becomes:

Figure 2.1 Path Constraint Example

Objective Function and Constraint Function vs. Control



Choose:

$$y = [u^1, t^1, u^2, t^2, \dots, u^i, t^i, \dots, t^{NCI-1}, u^{NCI}, t_f]^T \quad (2.13)$$

To minimize:

$$I(y) = F(x(t_f)) \quad (2.18)$$

Subject to:

$$\dot{x} = f(x, u, t); x(0) \text{ given} \quad (2.1)$$

$$[u_{\min}^1, 0, u_{\min}^2, 0, \dots, u_{\min}^{NCI}, 0]^T \leq y \leq [u_{\max}^1, t_{\max}, u_{\max}^2, t_{\max}, \dots, u_{\max}^{NCI}, t_{\max}]^T \quad (2.51)$$

$$[0, 0, 0, \dots]^T \leq [t^2 - t^1, t^3 - t^2, \dots, t_f - t^{NCI-1}]^T \leq [t_{\max}, t_{\max}, \dots, t_{\max}]^T \quad (2.52)$$

$$g_{\min} \leq g(x(t_f), u(t_f), t_f) \leq g_{\max} \quad (2.4)$$

Vectors y and l have dimensions $(nc + 1)NCI$ and $(NCI-1)$ respectively and these are reduced by one for the fixed end time problem. Constraint (2.52) ensures that the switching times remain ordered. Matrix l_y simply consists of elements 0, 1, or -1. $I(y)$ and $nl(y)$ are evaluated at t_f after a forward integration of the augmented state differential equations. Finally, the gradient matrices, I_y and nl_y , are determined from the backward integration of the adjoint systems given by Eq.(2.21) - (2.24) and Eq.(2.25) - (2.29) respectively.

The vector of non-linear constraints, $g(x(t_f), u(t_f), t_f)$, could be lumped together, in a manner similar to that used for path constraints, to form a single final time non-linear equality

constraint. Define:

$$g_o(x(t_f), u(t_f), t_f) = (g_{\min} - g)^T W_1 (g_{\min} - g) + (g - g_{\max})^T W_2 (g - g_{\max}) \\ = 0 \quad (2.53)$$

where W_1 and W_2 are $p \times p$ matrices chosen analagously to those given by Eq.(2.31) - (2.34). This reduces the number of adjoint systems connected with the non-linear constraints from p to 1. However, since this type of constraint represents a virtually unexplored area of non-linear programming, for the purposes of this work, the more general case of a p dimensional vector of non-linear constraints will be considered.

2.3 Structural Analysis and Computational Aspects of Optimal Control Problems

The approach to the optimal control problem now seems obvious. System equations are integrated forward to obtain values of the constraint and objective functions followed by gradient evaluation through the backward adjoint integration. Before this is blindly transformed into an optimal control package, it may be worthwhile to examine the problem structure for any features that could lead to computational savings. For most systems, the majority of computer time is spent on calculating the objective and constraint functions and gradients which suggests that the integration procedure itself plays a role of primary importance. Many chemical engineering operations are characterized by a set of stiff system equations, and thus any algorithm that is developed should certainly possess the capability of treating this class of problem.

2.3.1 The Problem of Stiffness

Consider the system of differential equations given by Eq.(2.1).

If the eigenvalues of the Jacobian matrix, f_x , are widely spread, then the system is considered stiff. For any explicit integration method, the step size is limited by the magnitude of the largest eigenvalue. The well known rule for Euler integration is an example. The step size, h , is given by:

$$h < \frac{2}{|\lambda|_{\max}} \quad (2.54)$$

where $|\lambda|_{\max}$ is the largest magnitude of the eigenvalues. However, the period of interest (e.g. a transient) is of the order $1/|\lambda|_{\min}$, and therefore many steps are needed to cover the transient region which results in a costly integration. The degree of stiffness in a system is expressed by the stiffness ratio, S , which is defined as:

$$S = \frac{|\lambda|_{\max}}{|\lambda|_{\min}} \quad (2.55)$$

In distillation operations, it is not uncommon to discover stiffness ratios ranging from 10^1 to 10^4 (Tyreus et al., 1975).

Most integration algorithms are synthesized by truncation of Taylor series expansion about a point. The resulting truncation error prevents the numerical solution from being exactly equal to the analytical solution. A method is said to be of order p if the local truncation error is proportional to h^{p+1} . Obviously one of the main objectives of the numerical analyst is to design methods with the highest possible order, but there are certain other properties which good numerical procedures should possess. A method is said to be convergent if, as $h \rightarrow 0$, the calculated solution approaches the actual solution. If the error propagated

in the integration procedure damps to zero as the number of integration steps approaches infinity, then the method is said to be absolutely stable. Stability analysis provides estimates of h that will satisfy this condition, and Eq.(2.54) is the result of such an analysis for the Euler formula.

An important class of integration methods, with applications in stiff systems, is the class of linear multistep methods. The general k -step method is given by:

$$\sum_{j=0}^k \alpha_j x_j = h \sum_{j=0}^k \beta_j f_j \quad (2.56)$$

where α_j and β_j are scalars. Euler's rule is a special case of Eq.(2.56) with $k = 1$, $\alpha_0 = -1$, $\alpha_1 = 1$, $\beta_0 = 1$, $\beta_1 = 0$. By setting $k = 1$, $\alpha_0 = -1$, $\alpha_1 = 1$, $\beta_0 = \frac{1}{2}$, $\beta_1 = \frac{1}{2}$, the familiar trapezoidal rule, given by:

$$x_k = x_{k-1} + \frac{h}{2} (f_k + f_{k-1}) \quad (2.57)$$

is obtained.

For stiff systems, the basic difficulty is to obtain suitably large stability regions, as demonstrated by the following definition and theorem by Dahlquist (1963).

Definition 2.1: A numerical method is said to be A-stable if its region of absolute stability contains the whole of the left-hand half-plane $\text{Re}(h\lambda) < 0$.

Theorem 2.1:

- (i) An explicit linear multistep method cannot be A-stable.
- (ii) The order of an A-stable linear multistep method cannot exceed 2.
- (iii) The second order A-stable implicit linear multistep method

with the smallest error constant is the trapezoidal rule. These are indeed severe restrictions. Higher order integration methods are desirable since lower truncation errors result but such procedures can only be implemented at the expense of loss of stability. In an effort to specify more relaxed conditions researchers have proposed $A(\alpha)$, $A(0)$, (Widland, 1967) and stiffly-stable (Gear, 1971) methods which define stability sections of the $h\lambda$ plane.

Part (i) of Theorem 2.1 is also numerically disappointing. A -stability implies implicitness and implicitness implies lengthy computation. Consider the following step generated by the general linear multistep formula:

$$x_k = h\beta_k f_k + b_k \quad (2.58)$$

where b_k is the known vector consisting of state and function values from previous steps. Since f_k is dependent on x_k , Eq.(2.58) is implicit and its solution is found usually by employing a non-linear equation solver. For example, application of a Newton method to Eq.(2.58) yields:

$$x_k^{[s+1]} - x_k^{[s]} = [I - h\beta_k f_{x_k}^{[s]}]^{-1} [x_k^{[s]} - h\beta_k f_k^{[s]} - b_k] \quad (2.59)$$

where superscript s refers to the successive iteration number. Convergence for the Newton method is usually obtained if a good initial estimate, supplied by a separate predictor, is employed. However, the calculation of $[I - h\beta_k f_{x_k}^{[s]}]^{-1}$ at each iteration can become tedious, especially for large systems. Sometimes the same estimate of the inverse is used for successive steps or advantage is taken of sparseness or special structure (e.g.

tridiagonal) of the Jacobian (Robertson, 1976) to facilitate a fast inverse evaluation.

Many methods have been proposed for solving stiff systems of equations. A survey by Bjurel et.al. (1970) reports on over forty methods, but obviously not all of these can be discussed here. Instead, the emphasis will be placed upon the computational savings realized from exploiting the structure of the resulting optimal control problem once the procedure has been implemented. The more general problem of comparing numerical methods for solving stiff differential equation systems is left to the numerical analyst and the interested reader is referred to an article by Enright et.al. (1975). For the purposes of this work, the proven Liniger-Willoughby method (1970) will be adopted. Burkett (1977) found that it performed extremely well for adsorption column applications and similar behaviour has been reported for distillation dynamics (Tyreus et. al., 1975). Since this algorithm falls into the general linear multistep class, any structural advantage gained can also be achieved from other methods belonging to this class (e.g. Gear's method).

The general form of the Liniger-Willoughby algorithm is stated as:

$$x_k = x_{k-1} + h[(1 - \mu)f_k + \mu f_{k-1}] \quad (2.60)$$

where μ , a parameter which is "exponentially fitted", is selected according to:

$$\mu = \frac{1}{h|\lambda_0|} - \frac{1}{e^{h|\lambda_0|} - 1} \quad (2.61)$$

The quantity λ_0 is the real part of the eigenvalue of the Jacobian matrix such that:

$$|\lambda_j - \lambda_0| \leq 1 \quad \text{for all } h|\lambda_j| > 1, \quad j = 1, 2, \dots, n \quad (2.62)$$

For distillation systems, Tyreus et.al. (1975) found that:

$$\lambda_0 = .5|\lambda|_{\max} \quad (2.63)$$

produced good results. The eigenvalue of maximum magnitude can be easily estimated from the well known Gerschgorin theorem:

$$|a_{ii} - \lambda_i| < \sum_{j=1, j \neq i}^n |a_{ij}| \quad (2.64)$$

where a_{ij} is the element of the i th row and j th column of the $n \times n$ Jacobian matrix. Obviously, as the Jacobian matrix changes over the trajectory, the exponential fitting parameter, μ , should be re-evaluated.

Liniger and Willoughby showed that Eq.(2.60) is A-stable if and only if $\mu < \frac{1}{2}$. Setting $\mu = \frac{1}{2}$ results in the special case of the trapezoidal rule, which has order 2. Otherwise, the Liniger-Willoughby algorithm has order unity.

2.3.2 Development of an Efficient Integration Method for Optimal Control Problems

The sets of differential equations for the reduced optimal control problem can now be examined in the light of integration methods for stiff systems. In review, the system, objective function adjoint and constraint function adjoint equations are given by:

$$\dot{x} = f(x, u, t) \quad ; \quad x(0) \text{ given} \quad (2.1)$$

$$\dot{\lambda} = -f_x^T \lambda ; \quad \lambda(t_f) = F_x^T \quad (2.23)$$

$$\dot{\lambda}_1 = -f_x^T \lambda_1 ; \quad \lambda_1(t_f) = g_x^T \quad (2.25)$$

where λ_1 is an adjoint matrix in which each column is connected with a final state constraint. Immediately, it can be recognized that the Jacobian on the right hand sides of Eq.(2.23) and (2.25) could be utilised in the integration routine. However, it is the indirect use of the Jacobian that leads to the most significant computational savings. Consider the evaluation of the relaxation matrix in Eq.(2.59) for a linear multistep integration of the system. Define:

$$R = [I - h\beta f_x] \quad (2.65)$$

where R is an $n \times n$ matrix.

The same quantity for the reverse integration of Eq.(2.23) and (2.25) is:

$$R_1 = [I - h\beta f_x^T] = R^T \quad (2.66)$$

That is, the transpose of the relaxation matrix for forward integration is the relaxation matrix for the backward integration. In general, since the evaluation of R and R_1 represents the most time consuming portion of the integrations, the relationship given by Eq.(2.66) becomes extremely valuable.

Rather than calculate the relaxation matrix inverse, it is more efficient to solve a set of linear equations at each step (Bowdler et.al., 1966). Consider Eq.(2.59) rewritten as:

$$R\Delta x^{s+1} = j_1^s \quad (2.67)$$

where:

$$\Delta x^{s+1} = x^{s+1} - x^s \quad (2.68)$$

and,

$$j_1^s = x^s - h\beta f^s - b \quad (2.69)$$

Iteration proceeds on Eq.(2.67) until: $\Delta x^{s+1} \sim 0$. A step in the backward adjoint integration can similarly be expressed as:

$$R^T \Delta \lambda^{s+1} = j_2^s \quad (2.70)$$

The standard Crout decomposition performed on R is given as:

$$R = LU \quad (2.71)$$

Where L is a lower triangular matrix and U is an upper triangular matrix with a unit diagonal. In order to avoid numerical instabilities during the decomposition, partial pivoting should be used (Wilkinson and Reinsch, 1971). Let K_{pi} denote the matrix, whose multiplication of R gives an interchange of the *i*th and *p*th rows of R. Thus, partial pivoting results in:

$$K_{pn} K_{p(n-1)} \cdots K_{p1} K_{p2} R = KR = \tilde{R} = LU \quad (2.72)$$

(i.e. Crout decomposition of $\tilde{R}$)

Premultiplication of Eq.(2.67) by K yields:

$$KR \Delta x^{s+1} = K j_1^s \quad (2.73)$$

Substituting the equivalent value of KR from Eq.(2.72) into Eq.(2.73) gives:

$$LU \Delta x^{s+1} = K j_1^s \quad (2.74)$$

The following simpler problems are then solved by successive substitution:

$$Lz = K j_1^s \quad (2.75)$$

$$U\Delta x^{s+1} = z \quad (2.76)$$

Therefore, once the $\tilde{R}$ matrix is decomposed and j_1^s is subjected to the appropriate row interchanges, the two problems can be solved to yield the solution.

Now consider a backward integration step given by Eq. (2.70). Since $(\kappa_{pi})^{-1}$, $i = 1, 2, \dots, n$ exist, $(K^T)^{-1}$ exists, then Eq.(2.70) can be rewritten as:

$$R^T K^T (K^T)^{-1} \Delta \lambda^{s+1} = j_2^s \quad (2.77)$$

or:

$$U^T L^T (K^T)^{-1} \Delta \lambda^{s+1} = j_2^s \quad (2.78)$$

The solution to Eq.(2.70) is equivalent to the solution of the following simpler problems:

$$U^T z_1 = j_2^s \quad (2.79)$$

$$L^T z_2 = z_1 \quad (2.80)$$

$$\Delta \lambda^{s+1} = K^T z_2 \quad (2.81)$$

Further simplifications can be achieved by examining the properties of the K matrix. It is clear that:

$$\kappa_{pi}^T = \kappa_{pi} \quad (2.82)$$

and therefore Eq.(2.81) can be simplified to give:

$$\Delta \lambda^{s+1} = \kappa_{p1} \kappa_{p2} \dots \kappa_{pn} z_2 \quad (2.83)$$

Note that the backward adjoint integration step is solved by implementing the transpose of the decomposition matrices for the forward integration. The row interchange procedure that ensured stability of the decomposition algorithm is applied in reverse via Eq.(2.83) to arrive at the solution to the adjoint equation.

It must be stressed that Eq.(2.67) and (2.70) represent one iteration at one step of the integration. How many iterations are needed at each step to ensure convergence? How many steps can be taken before the decomposition matrices must be updated? How much reduction in computer time, if any, can be expected in comparison with standard integration methods? The following numerical example will attempt to answer these questions.

2.3.3 Numerical Example

The integration method proposed in the previous section was tested on the splitter model which is outlined in section 3.1.2. Basically, the model consists of 28 different equations which describe compositions and flowrates throughout the column. The equations are not stiff, having a stiffness ratio of approximately 40 in the region of interest. An objective function that measures the deviation from final set point of light component at selected column locations is used. It has the form:

$$I = \int_0^{t_f} \{(C_{1D} - .6561)^2 + (C_{1S} - .2300)^2 + (C_{1B} - .0242)^2\} dt \quad (2.84)$$

where: C_{1D} is the composition of the light component in the distillate,

C_{1S} is the composition of the light component in the sidestream,

C_{1B} is the composition of the light component in the bottoms.

Accurate integration procedures are required to furnish an accurate value of the objective function for a given control trajectory.

If an exact value of I can be determined, any deviation would be representative of integration error.

The splitter model was established to simulate a change in state over 2.1 hours with 3 control variables, 4 control intervals and no terminal time constraints. In order to provide a realistic example for the tests, the controls were changed over 9 iterations of VMP where a Runge-Kutta method was implemented to evaluate the objective function and gradients. The resulting controls were used for the test case.

The corresponding adjoint system will have dimension 29. Any inaccuracies in the reverse adjoint integration will be accumulated in the first control interval and therefore G_{1R} , the gradient of the objective function with respect to the reflux control in the first control interval, has been taken as a measure of the adjoint integration performance.

The system equations and adjoints were integrated using the linear multistep formula given in Eq. (2.60). The predictor:

$$x_{k+1} = \frac{h}{2} f_k \quad (2.85)$$

gave a first estimate at each step. For each integration the following parameters must be specified:

STEP - the integration step size

NJUP - number of integration steps between decomposition matrix updates

NCONV - number of iterations for convergence at each step

μ - the fitting parameter

The values of the state at each step were stored on disc so that the Jacobian matrix could be evaluated at each step of the backward integration. Similar storage was provided for the decomposition matrices at every NJUP steps. It should be noted that these

matrices are automatically updated at each new control interval since this is when the most violent changes in state usually occur.

Table 2.1 shows values of I and G_{1R} using a Liniger-Willoughby integration for various NJUP and NCONV. Note that the decomposition matrices performed very robustly. Integrations with NJUP = 50 (i.e. one update per control interval) give results within 0.5% of those with NJUP = 25 (i.e. two updates per control interval). Two convergence iterations ensure sufficient accuracy on the forward integration whereas only one is necessary for the adjoint system. The latter observation is not surprising since it is known that the Newton method is known to converge in one iteration for linear systems. (Sarkany and Liniger, 1974). Although the adjoint system represented by Eq.(2.23) is influenced by the time varying Jacobian, the sensitivity of the convergence procedure to the frequency of Jacobian updates for the relaxation matrix appears to be small.

Using NJUP = 50, NCONV = 2 for the system equations, NCONV = 1 for the adjoints, trapezoidal rule integrations were performed for various step sizes. These results are shown in Table 2.2. Table 2.3 illustrates the effect of step sizes on the objective function for a fourth order Runge-Kutta method. Note that the stability limit for this routine occurs at $h < 0.1$ whereas the trapezoidal procedure integrated stably at step sizes over four times higher than this value.

Total computation time for the runs can be estimated from the times required to execute the major subroutines which are shown in Table 2.4. Figure 2.2 demonstrates the trends in the relationship between objective function accuracy and total CDC 6400 computation

TABLE 2.1 VALUES OF I AND G₁R FOR VARIOUS NJUP AND NCONV

h = 0.014 hr.
μ - exponentially fitted

NCONV	NJUP			
	25		50	
	I	G ₁ R	I	G ₁ R
1	.839066099E-03	-.264378264E-03	.838139896E-03	-.265271352E-03
2	.915372519E-03	-.263322118E-03	.915477864E-03	-.263277440E-03
3	.9136406569E-03	-.263387959E-03	.913622656E-03	-.263386438E-03

Note: E-x = 10^{-x}

TABLE 2.2 VALUES OF I AND G1R FOR VARIOUS STEP SIZES

NJUP = 50
NCONV = 2, forward integration
NCONV = 1, backward integration
 $\mu = \frac{1}{2}$

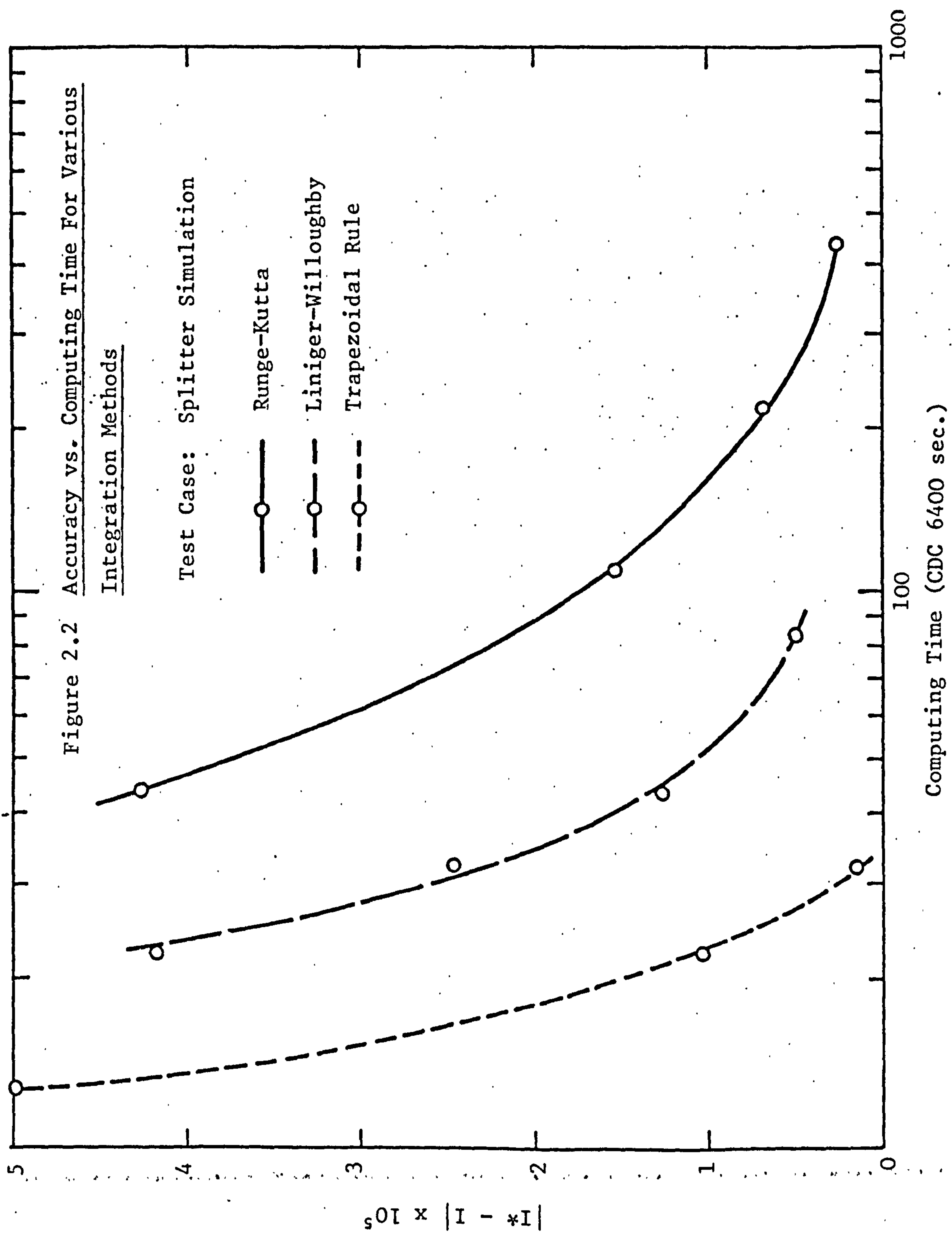
h (hr.)	I	G1R
.042	.991369903E-03	-.248017296E-03
.021	.950610636E-03	-.263821139E-03
.014	.941340343E-03	-.266909785E-03

TABLE 2.3 VALUES OF I FOR RUNGE-KUTTA INTEGRATIONS

h (hr.)	I
.01	60.6228773
.005	.982659052E-03
.002	.95572237E-03
.001	.946759011E-03
.0005	.942682285E-03

TABLE 2.4 COMPUTING TIMES FOR THE MAJOR SUBROUTINES IN THE
INTEGRATION PROGRAM

Routine	Purpose	Average Computing Time (CDC 6400 sec.)
CYSTEEM	Evaluates RHS of State Equations	.003
JACBX	Evaluates Jacobian of State Equations	.023
DECOMP	Decomposes relaxation matrix into $\hat{K} = LU$	.613
SOLIN	Solves the set of Linear Equation $KR\Delta x = K j_1$	.048



time for the three integration methods. The accurate value of the objective function was found by extrapolating the Runge-Kutta results to $h = 0$ which yielded $I^* = .9398E-03$. In the analysis of the total computing time, it was assumed that four function evaluations were used at each Runge-Kutta step in the forward and reverse integrations. For the other two methods, calculations were based on $NJUP = 50$, $NCONV = 2$ for the system equations and $NCONV = 1$ for the adjoints.

The savings in computer time resulting from reuse of the decomposition matrices in linear multistep methods are now evident. For this problem, the trapezoidal rule proved to be approximately twice as fast as the exponential fitting method for a given accuracy and this can be expected since the model equations are not stiff. Both these methods were superior to the Runge-Kutta integration showing up to a tenfold decrease in computing time for the same error tolerance. If the system equations are stiff, the trapezoidal rule and exponential fitting procedure may exchange positions in Figure 2.2, but they will certainly still outperform Runge-Kutta methods by at least the same degree. Furthermore, the integration of adjoints corresponding to final state constraints would produce additional computing time reduction resulting from application of the same decomposition matrices.

In the cases where optimal control acts as a tool to synthesize control systems, the investment of a very accurate integration must be questioned. For example, from Figure 2.2, an objective function error of 2×10^{-5} could probably be tolerated without seriously affecting the optimal control trajectory. In fact, one could envisage an algorithm whereby the stepsize is controlled to

be large when the optimization begins, gradually progressing to the smallest allowable stepsize as convergence proceeds.

2.4 An Algorithm for Optimal Control Problems

The integration methods presented in the previous section will form the basis of a numerically efficient optimal control algorithm. Considerable computational savings are realized because decomposition matrices used on the forward integration can be exploited on the reverse integration where the gradients are calculated. Normally, non-linear programs only require gradients after the objective or non-linear constraint functions have been evaluated. Non-linear constraint functions are always determined at the same point as the objective function but not necessarily vice versa. When a step in the optimization results in constraint violation, the non-linear constraint function and gradients are required to regain feasibility. The following free end-time algorithm begins after the optimization driving routine has called for objective and non-linear constraint functions with their respective gradients, and the extension to any subset of this combination is obvious. It assumes that values of h , NCI , $NJUP$ and $NCONV$ have been established in the main program.

1. Set $i = 1$, $t^0 = 0$, $x(t^0) = x(0)$
2. Evaluate f_x . Set $\mu, \tilde{R}$ (cf. Eq.(2.61), (2.72))
3. Integrate $\dot{x} = f(x, u^i, t)$ from t^{i-1} to t^i , iterating $NCONV$ times at each step. Store x (on disk) at each step. At each $NJUP$ steps, update and store $\tilde{R}$ and μ (on disk).
4. Store $G^i = f(x(t^i), u^i, t^i) - f(x(t^i), u^{i+1}, t^i)$ if $i < NCI$.
Otherwise evaluate $G^i = f(x(t_f), u^{NCI}, t_f)$

5. Set $i = i + 1$. If $i < \text{NCI}$ go to STEP 2. Otherwise evaluate $F(x(t_f))$, $g(x(t_f), u^{\text{NCI}})$, $\{F_x, g_u, g_x, g_t\}_{t=t_f}$
6. Set $i = \text{NCI}$, $\lambda(t_f) = F_x^T$, $\lambda_1(t_f) = g_x^T$, $C_1 = g_u$. Evaluate $F_{t_f} = \lambda^T(t_f)G^i$, $g_{t_f} = g_t + \lambda_1(t_f)G^i$
7. Set $z_1 = \lambda^T f_u(x(t_i), u^i, t^i)$, $z_2 = \lambda_1^T f_u(x(t_i), u^i, t^i)$, $z_3 = z_4 = 0$. If $i < \text{NCI}$, set $C_1 = 0$
8. Integrate $\dot{\lambda} = -f_x^T \lambda$, $\dot{\lambda}_1 = -f_x^T \lambda_1$ from t^i to t^{i-1} , iterating once at each step. Values of f_x are calculated from stored x values. R and λ are retrieved from storage so that they may be used over the same integration steps as in the forward direction. At each step, calculate $z_3 = z_3 + \frac{1}{2}(\lambda^T f_u + z_1)$
 $z_4 = z_4 + \frac{1}{2}(\lambda_1^T f_u + z_2)$. Set $z_1 = \lambda^T f_u$, $z_2 = \lambda_1^T f_u$
9. Evaluate $F_{ui} = -z_3$, $F_{ti} = \lambda^T(t_i)G^i$, $g_{ui} = C_1 - z_4$, $g_{ti} = \lambda^T(t_i)G^i$.
10. Set $i = i - 1$. If $i > 0$, go to STEP 7. Otherwise RETURN to optimization routine.

Note that the trapezoidal rule was used to integrate Eq.(2.21) and (2.27) simultaneously with the adjoints. Since these are simply time varying functions, and the adjoint trajectories are known, any other standard method (e.g. Simpson's) could have been implemented.

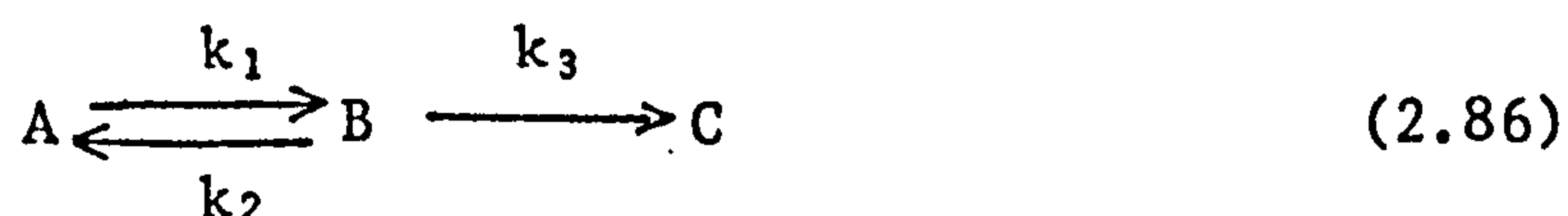
The implicit integration algorithm for the states and adjoints assumes no special structure of the Jacobian matrix, f_x . Naturally, if such a structure does exist, the algorithm should be modified to exploit it. For example, it is well known that for a binary distillation column with theoretical plates, a tri-diagonal Jacobian results, whose inverse is easy to evaluate. Tyreus et.al. (1975) demonstrate how this effects a rapid Liniger-

Willoughby integration. Also, routines are available (Curtis and Ried, 1971) to solve the set of linear equations at each iteration, given by Eq.(2.45) and (2.48), when matrix R is sparse.

A computer package based on this algorithm would only require the user to supply Fortran subroutines to evaluate $f, f_x, g_u, g_t, f_u, F, F_x, g, g_x$ for given values of x, u , and t . The main problem for the potential user would be to specify the number of control intervals, NCI . A large number of control intervals could approximate a continuous control signal at the expense of large storage and lengthy computation. Alternatively, a small value of NCI would converge rapidly to a piecewise solution of the reduced problem. Ideally, one would desire a changing NCI policy in which large time intervals of constant controls were utilized to facilitate initial changes in the objective function, after which NCI would be gradually increased to converge to a solution of the original problem. As a result of applications to measurement subset selection, Mellefont (1977) demonstrates the implementation of changing NCI policies in conjunction with the above algorithm for the bounded control case.

2.4.1 Numerical Example

In order to test the algorithm, consider the well known problem of mixed catalysts for successive reactions in a tubular reactor, given by the following reaction scheme (Gunn and Thomas 1965; Thomas and Wood, 1967; Jackson, 1968; Nishida et al., 1976):



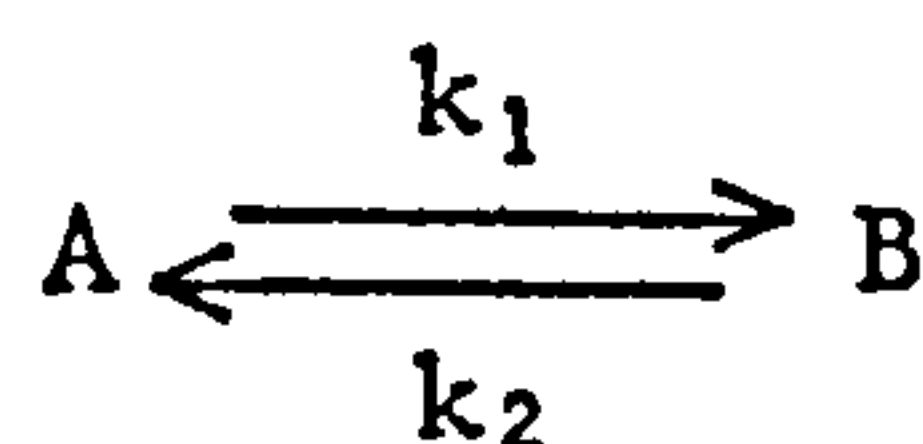
Let the mole fractions of A and B be denoted by x_1 and x_2 respectively. The differential equations which describe the composition

trajectories along the reactor length are:

$$\dot{x}_1 = u(k_2x_2 - k_1x_1) \quad (2.87)$$

$$\dot{x}_2 = u(k_1x_1 - k_2x_2) - (1 - u)k_3x_2 \quad (2.88)$$

where t is the residence time of substance from the instant of entry to the reactor and u is the fraction of catalyst which catalyses the reaction:



It is assumed that u can be varied along the reactor length, with the obvious physical constraint:

$$0 \leq u(t) \leq 1 \quad (2.89)$$

The optimal control problem is to determine, $u(t)$, to maximize the outlet concentration of C, or to minimize the outlet concentration of the other two components. Thus, the objective function is given by:

$$F = x_1(t_f) + x_2(t_f) \quad (2.90)$$

The control appears linearly in Eq.(2.87) and (2.88) and from Pontryagin's Maximum Principle, bang-bang control could be expected. However, because of the bilinear coupling of the states and controls in the system equations, singular arcs (with control not on its bounds) may exist.

The value of the final time and reaction rate constants are chosen to be the same as those used by Gunn and Thomas (1965), Jackson (1968), and Nishida et al. (1976). Namely, $t_f = 1.0$, $k_1 = k_3 = 1.0$, $k_2 = 10$. The problem has been solved analytically by Jackson (1968) using phase plane analysis with the maximum principle and a singular arc does result. This is not surprising since bang-bang control

can be interpreted as performing the conversion in two successive reaction steps using two separate reactors.

The optimal control algorithm developed previously was coded into a Fortran package (OPCON). The mixed catalyst problem was coded for OPCON using the following information:

$$f_x = \begin{bmatrix} -k_1u, k_2u \\ k_1u, -k_2u + k_3u - k_3 \end{bmatrix} \quad (2.91)$$

$$f_u = \begin{bmatrix} k_2x_2 - k_1x_1 \\ k_1x_1 - k_2x_2 + k_3x_2 \end{bmatrix} \quad (2.92)$$

$$F = x_1 + x_2 \quad (2.93)$$

$$F_x = \begin{bmatrix} 1 & 1 \end{bmatrix} \quad (2.94)$$

An initial starting guess of $u = 0.2$, $0 \leq t \leq 1$, was used. NCI was set to 5 with switching times at 0.2, 0.4, 0.6, and 0.8.

After 17 iterations (21 objective function evaluations) OPCON produced the control trajectory shown in Figure 2.3. In the same figure, Jackson's analytical solution and the resulting policy of the modified Max-H algorithm of Nishida et al. are given.

Note that OPCON has moved control levels and paired switches so as to almost duplicate the analytical solution. The optimal

outlet concentration of C for the analytical solution is .048065

compared with .048059 from OPCON after 14 seconds of CDC 6400 computing time. The Max-H strategy took 25 iterations and 15 seconds

of IBM 370/155 computer time (~ 22 seconds CDC 6400) to achieve the

shown control policy. Nishida et al. (1976) state that their results

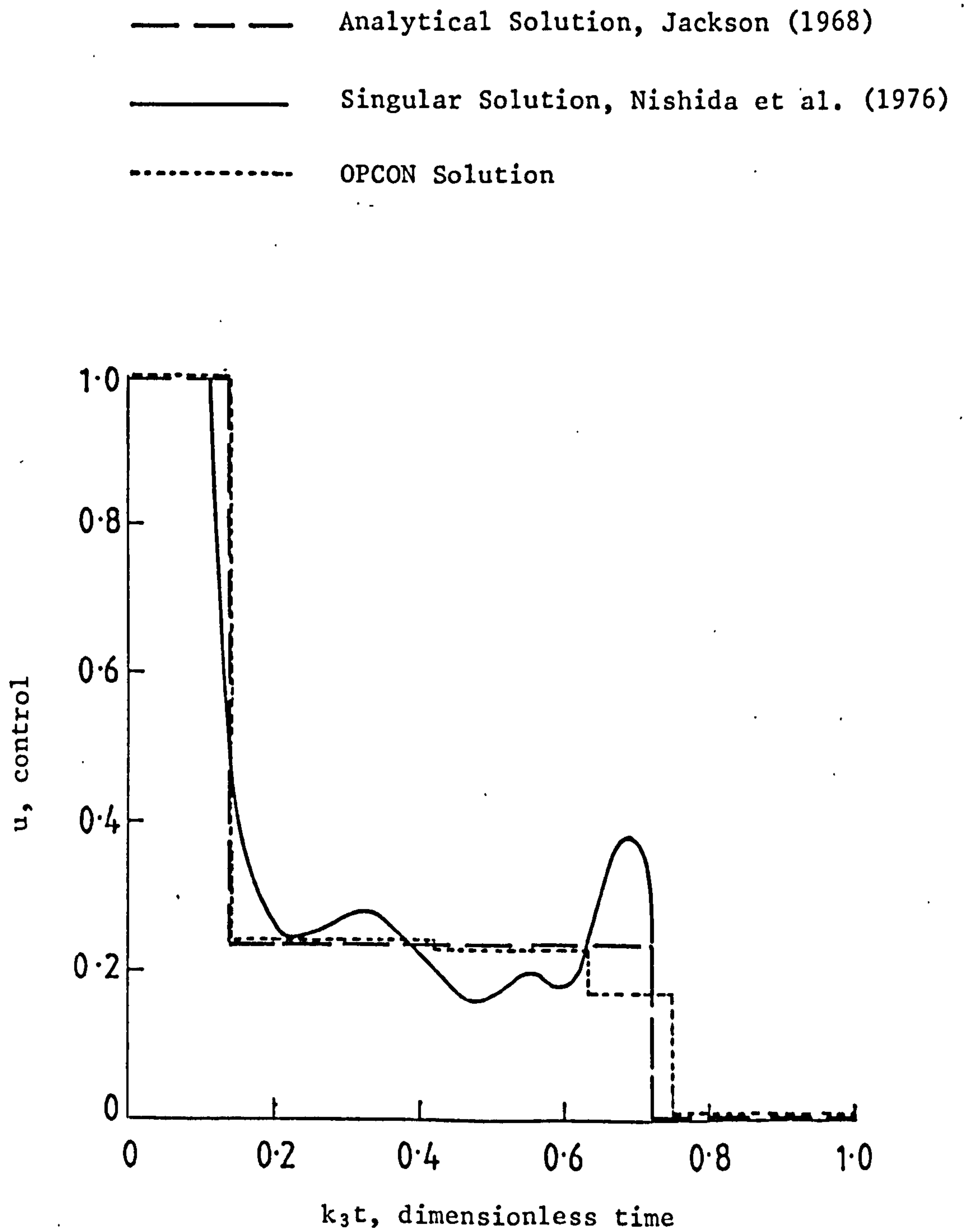
compare favourably with gradient and second variation techniques

in that these methods cannot obtain the large changes in the

control quickly enough to assure rapid convergence. Since OPCON

outperforms the Max-H algorithm, its efficiency is self evident.

Figure 2.3 Control Signal Comparison for Mixed Catalyst Problem



Nishida et al. also apply a pure bang-bang policy as a sub-optimal approximation to the optimal control. Although the states almost follow the optimal trajectory, the resulting bang-bang control would be difficult to implement since it implies successive layers of each catalyst. For the purposes of this work, both the states and controls are of interest and bang-bang control generally represents too harsh a solution for refinery implementation. Therefore, an algorithm capable of approximating the singular trajectory is a necessity.

CHAPTER 3 - FORMULATION OF FEED CHANGEOVERS AS OPTIMAL
CONTROL PROBLEMS

3.1 Dynamic Models for Distillation Processes

Distillation is a non-linear process. The choice of model to represent the column dynamics should reflect the range of operation and purpose of the model. For accurate off-line transient responses, detailed plate-to-plate calculations may be used. Alternatively, on-line applications for feedforward and direct digital control demand a much simpler model, preferably one which could be updated as the operating region changes. These two extremes of model sophistication will be examined in turn, followed by a discussion of suitable models for optimal control. The reader interested in a detailed discussion of dynamic models for distillation is referred to a recent comprehensive review by Rademaker et al. (1975).

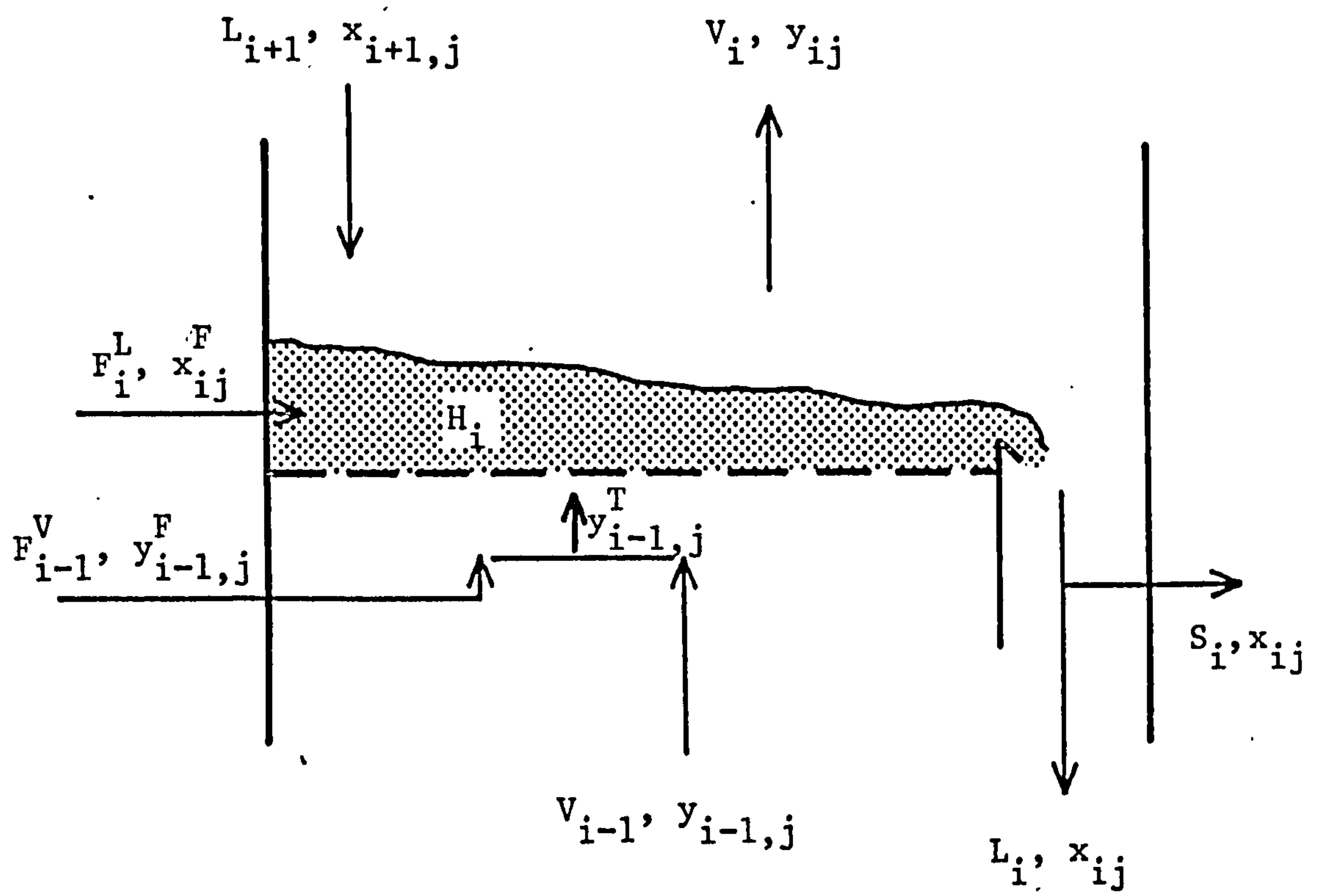
Luyben (1973) has presented a general N component dynamic distillation column model with non-ideal vapour liquid equilibrium, inefficient trays, and variable pressures. Refer to Fig. 3.1. By assuming perfect liquid mixing on each plate, negligible tray vapour holdups, and thermal equilibrium, he arrived at the following set of equations for the i th tray:

$$\frac{dH_i}{dt} = L_{i+1} + F_i^L + F_{i-1}^V + V_{i-1} - V_i - L_i - S_i \quad (3.1)$$

Component mass balance equation ($N - 1$ per tray):

$$\begin{aligned} \frac{d}{dt} (H_i x_{ij}) = & L_{i+1} x_{i+1,j} + F_i^L x_{ij}^F + F_{i-1}^V y_{i-1}^F \\ & + V_{i-1} y_{i-1,j} - V_i y_{ij} - L_i x_{ij} - S_i x_{ij} \end{aligned} \quad (3.2)$$

Figure 3.1 i th Tray of Multicomponent Distillation
Column Showing j th Component Distribution



Energy (one per tray):

$$\begin{aligned} \frac{d}{dt} (H_i U_i) = & L_{i+1} h_{i+1} + F_i^L h_i^F + F_{i-1}^V Y_{i-1}^F + V_{i-1} Y_{i-1} - V_i Y_i \\ & - L_i h_i - S_i h_i \end{aligned} \quad (3.3)$$

Murphee tray efficiency (N - 1 per tray):

$$E_{ij} = \frac{y_{ij} - y_{i-1,j}^T}{y_{ij}^* - y_{i-1,j}^T} \quad (3.4)$$

Phase Equilibrium (N per tray):

$$y_{ij}^* = f(x_{i1}, x_{i2}, \dots, x_{iN}, P_i, T_i) \quad (3.5)$$

Thermal Properties:

$$h_i = f(x_{i1}, x_{i2}, \dots, x_{iN}, T_i) \quad (3.6)$$

$$Y_i = f(y_{i1}, y_{i2}, \dots, y_{iN}, T_i, P_i) \quad (3.7)$$

$$h_i^F = f(x_{i1}^F, x_{i2}^F, \dots, x_{iN}^F, T_i^F) \quad (3.8)$$

$$Y_i^F = f(y_{i1}^F, y_{i2}^F, \dots, y_{iN}^F, T_i^F, P_i) \quad (3.9)$$

Tray Hydraulics:

$$L_i = f(x_{i1}, x_{i2}, \dots, x_{iN}, H_i, V_i, T_i, P_i, S_i) \quad (3.10)$$

$$V_i = f(P_i, P_{i-1}, y_{i1}, y_{i2}, \dots, y_{iN}, T_i) \quad (3.11)$$

Where:

H_i is the liquid holdup of the i th tray

F_i^L is the liquid feed rate to the i th tray

F_{i-1}^V is the vapour feed rate to the $i-1$ tray

V_i is the vapour rate of the i th tray

S_i is the liquid drawoff rate from the i th tray

- x_{ij} is the liquid mole fraction of the j th component on the i th tray
- x_{ij}^F is the liquid mole fraction of the j th component in the feed to the i th tray
- y_{ij} is the vapour mole fraction of the j th component on i th tray
- $y_{i-1,j}^F$ is the vapour mole fraction of the j th component in the feed to the $i-1$ tray
- $y_{i-1,j}^T$ is the actual vapour mole fraction of the j th component entering the i th tray
- y_{ij}^* is the vapour mole fraction of the j th component in phase equilibrium with liquid on the i th tray
- E_{ij} is the Murphee vapour efficiency for the j th component on the i th tray
- U_i is the total internal energy of the liquid on the i th tray
- h_i is the enthalpy of the liquid on the i th tray
- Y_i is the enthalpy of the vapour on the i th tray
- Y_{i-1}^F is the enthalpy of the feed vapour entering the $i-1$ tray
- h_i^F is the enthalpy of the feed liquid entering the i th tray
- T_i is the temperature of tray liquid and vapour
- T_i^F is the temperature of the feed entering the i th tray
- P_i is the pressure on the i th tray

Similar equations describe the behaviour of the condenser and reboiler. Assuming that the algebraic functions given by Eq.(3.4)-

(3.11) could be solved at each integration step, the model can be reduced to $N + 1$ ordinary differential equations for each tray. Refinery columns can have as many as sixty trays and for a five component distillation, this results in at least a 360 dimensional model. Using a 14 dimensional model representing a binary distillation system with non-linear equilibrium relationships, Distefano et al. (1967) found it took 12 minutes of IBM 7094 computing time to evaluate a single transient run. Obviously, such a model is impractical for on-line use and even the feasibility of off-line transient calculations for large multicomponent systems must be questioned.

Thus an incentive is provided to examine simpler models for distillation dynamics. A first approximation would be to include dynamics only as a variable affecting the steady state solution. Van der Grinten and Duyfjes (1973) incorporate a mass balance for a binary column to give:

$$\frac{x_F - x_B}{x_D - x_B} = \frac{D}{F} + c \quad (3.12)$$

where:

x_F is the light component feed composition

x_B is the light component bottoms composition

x_D is the light component distillate composition

D is the distillate flowrate

F is the feed rate

c is an updated term to account for imbalances or dynamic effects

This was coupled with Shinskey's (1967) separation equation:

$$S = \frac{x_D(1 - x_B)}{x_B(1 - x_D)} = a + b \frac{V}{F} \quad (3.13)$$

where

S is the separation factor

V is the column vapour rate

a, b are fitted parameters

Parameters a , b and c were estimated from plant data. Using optimal values of x_B and x_D , together with measured values of F and x_F , Eq.(3.12) and (3.13) were solved for controls D and V . Since this type of model only recognises the dynamics after their occurrence it would not suffice for off-line simulations where advance knowledge of the upsets could be useful.

In an attempt to simplify transient response predictions, several unifying criteria have been recommended. The concept of disturbance function was suggested by Rosenbrock (1960) in which the rate of change of the entire column holdup of light component for a binary separation was determined. However, the disturbance function has not been developed to the extent whereby column responses can be predicted from given upsets. Considerably more success has been obtained from the inventory time concept. The original inventory time as defined by Moczek et al. (1965) could be interpreted as a pseudo-first order time constant for the complete holdup of the column. Time constants for responses at both ends of a binary column were later derived by Bhat and Williams (1969) and Weigand et al. (1972). The latter authors introduced the method of minimal change of storage to decouple the interactions between the two time constants.

Unfortunately, the extension to multicomponent, multiproduct columns is not obvious and the response to multiple disturbances still remains a topic of research.

It is now apparent that the over sophistication of the plate-to-plate models together with the over simplicity of low order models indicates that a compromise between model accuracy and detail is necessary. The most popular approach is to linearize the non-linear dynamic and algebraic equations about an operating point and then to apply linear systems theory. Transfer function relationships for binary columns have been studied by Gilliland and Mohr (1963) and Whal and Harriott (1970). For control purposes, usually only the responses of product stream compositions rather than intermediate tray concentrations are of interest and therefore model reduction of linear systems may be utilized. Kim and Friedly (1974) developed techniques that enable any input-output response of large linear staged systems to be represented by a second order transfer function with dead time. Numerous accounts of successful applications of linear binary distillation models for optimal control appear in the literature (Rafal and Stevens, 1968; Brosilow and Handley, 1968; McGinnis and Wood, 1974; Oakley and Edgar, 1976).

However, for feed changeover studies, the mathematical convenience of linear models is offset by localization problems. If the model is linearized about the initial steady state, the model will not be valid when the process is driven far away from that state. Hu and Ramirez (1972) tested a non-linear binary model together with its linearized version for simultaneous 10% decreases in feed and reflux temperatures coupled with 10% increases in feed rate and composition. This resulted in as much as a 38%

difference between the predictions of the final steady state compositions. Such performances of linear models can seriously affect any gains derived from optimal control calculations. For example, Jacobs and Dyer (1975) implemented a linear model to determine the minimum variance regulator for a three product multicomponent distillation column. Identification experiments were performed about a single steady state but the action of the "optimal" controller required improvement in regions away from this state. The proposal of a sequence of linearized models covering state space would certainly increase the identification effort.

Other simplifications that circumvent the problems of linearization are sought. Osbourne et al. (1965) present a model for binary columns that lumps all the trays of the rectifying section together and likewise for the stripping section. Component balances for each section lead to ordinary differential equations in which mass transfer terms are estimated from steady state data. The total number of equations are reduced to one per component per section thus allowing rapid transient calculations. Experimental results have been reproduced with good accuracy and further work by Osborne and Maddox (1967) and by Burman and Maddox (1969) give good model performance in conjunction with a feedforward control algorithm. The extension to multicomponent multiproduct distillation columns simply requires additional sections between adjacent product or feed streams and the fact that the development to date has led to linear models does not prevent the introduction of non-linear terms in the describing differential equations. The combined advantages of low model order with accurate plant representation has resulted in BP developing

the sectional concept for the three columns considered in this work.

The simplest of these models, the debutanizer, represents a binary column and is basically used to gain confidence and experience with the optimal control package. Although it is not a particularly accurate model, it does successfully predict correct forms of column responses. The splitter and main column models are of almost identical structure except that the main column is represented by five product streams and pseudo components as opposed to three for the splitter. Since the splitter model is smaller and thus provides faster transient calculations, it was utilized to develop objective function formulations and product stream storage policies for the main column. These are discussed in subsequent sections. Most of the benefit, in terms of control, for the three column system is expected from the main column since it operates on five to eight times the throughput of each of the other two columns.

3.1.1 The Debutanizer

A schematic of the debutanizer illustrating the column sections is given in Fig. 3.2. Only the general philosophy of the model will be discussed here.

Eq.(3.13) is Shinskey's (1967) extension of the Fenske separation factor. It relates the steady state feed and vapour flowrates to a ratio of product stream composition functions. This can be coupled with a component mass balance to yield a quadratic equation in terms of product flowrates, feed flowrates and composition, and the separation factor. The solution is the steady state component composition in either the top or bottom

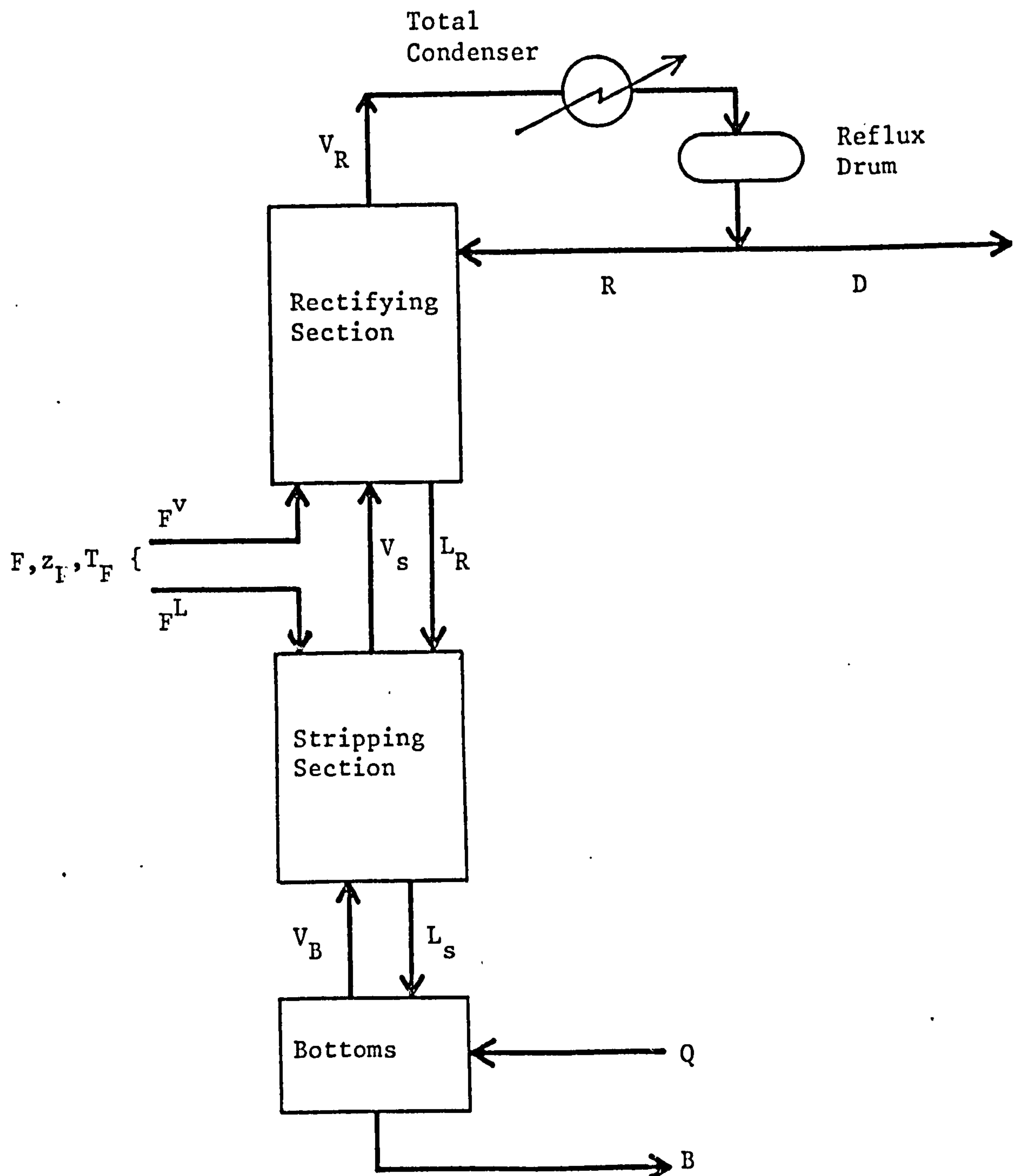


Figure 3.2 The Debutanizer

product. Extension to the dynamic case is as follows. Given initial conditions for flowrates and compositions, reflux and fuel rate trajectories, the liquid rates are derived from differential equations describing the time rate of change of section holdups. Column vapour rates are determined from functions of fuel rate. For each section, the feed rate and composition are lagged to simulate the effect on the product streams. These values together with the product flowrates and the instantaneous separation factor are substituted into two quadratic equations. The solutions represent the steady state composition of light and heavy component in the bottoms and top vapour respectively. Since steady state is not instantly achieved these concentrations are subjected to a further lag in order to obtain the time varying compositions. Stream temperatures are evaluated from linear functions of stream compositions.

In state space form, the model is characterized by a set of 10 differential equations. It is controlled by the reflux rate, R , and the fuel rate and is subjected to upsets in the feed rate, F , feed composition, z_F , and feed temperature, T_F . Product flow rates, D and B , are used to control levels in the reflux and reboiler drums respectively. The structure is in the form of:

$$\dot{y} = Ay + Bu + d \quad (3.14)$$

$$\dot{x} = Ex - f(y) \quad (3.15)$$

where y is the vector of lagged flowrates and feed compositions, u is the control vector, d is the disturbance vector, x is two dimensional product composition vector, and $f(y)$ represents the instantaneous quadratic solution.

3.1.2 The Splitter

The splitter model is based on a three component system with three product streams. Model sections are shown in Fig. 3.3. Associated with each section, there is a set of four differential equations describing the exit vapour rate, exit liquid rate, and exit liquid concentrations of the light and middle components. These are given by:

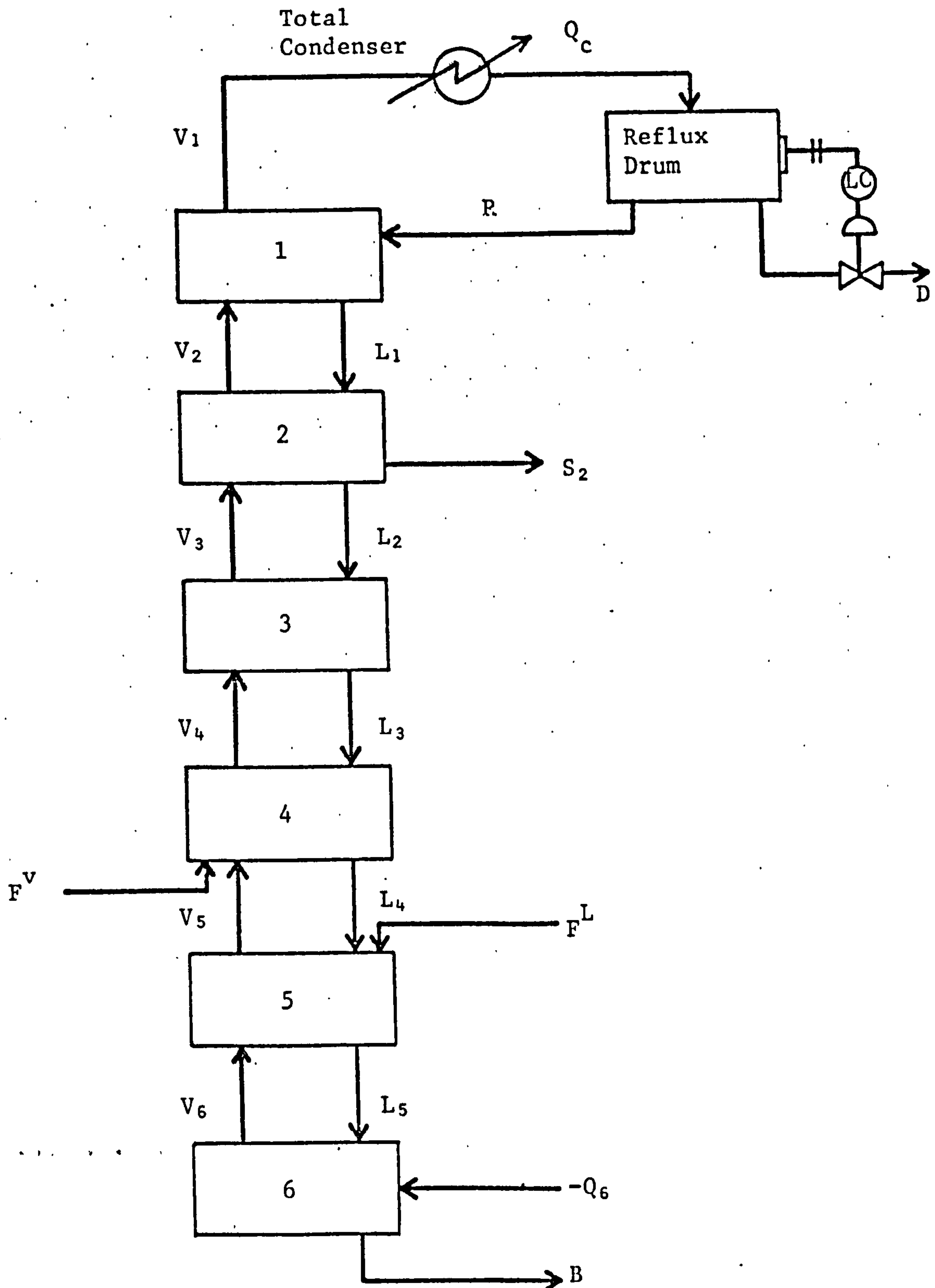
$$\begin{aligned} \frac{dV_{out}}{dt} = & \frac{1}{\tau_m} \left\{ (k - 1)(V_{in} - L_{in}) - \frac{kQ_{out}}{\lambda} - (V_{out} - V_{in}) \right\} \\ & + \frac{dV_{in}}{dt} \end{aligned} \quad (3.16)$$

$$\begin{aligned} \frac{dL_{out}}{dt} = & \frac{1}{\tau_H} \{ L_{in} - L_{out} + V_{in} - V_{out} \} + \frac{dV_{in}}{dt} - \frac{dV_{out}}{dt} \end{aligned} \quad (3.17)$$

$$\begin{aligned} \frac{dx_{out,j}}{dt} = & \frac{1}{H} \{ V_{in}(y_{in,j} - x_{out,j}) + L_{in}(x_{in,j} - x_{out,j}) \\ & - V_{out}(y_{out,j} - x_{out,j}) \} \end{aligned} \quad (3.18)$$

where:

- V_{in} is the total vapour flow into the section
- V_{out} is the total vapour flow out of the section
- L_{in} is the total liquid rate into the section
- L_{out} is the total liquid rate out of the section
- Q_{out} is the total external heat flow out of a section
- $x_{out,j}$ is the exit liquid composition of the jth component
- $x_{in,j}$ is the entering liquid composition of the jth component

Figure 3.3 The Splitter

$y_{out,j}$ is the exit vapour composition of the j th component

$y_{in,j}$ is the entering vapour composition of the j th component

H is the holdup, constant

λ is the latent heat of vaporization, constant

k, τ_m, τ_H are fitted parameters

The exit vapour compositions are expressed as:

$$y_{out,j} = f(x_{out,1}, x_{out,2}) \quad ; \quad j = 1, 2 \quad (3.19)$$

Assumptions used in the development of Eq.(3.16)-(3.18) are discussed in section 3.1.4.

Some control structure is implied by the level control system on the reflux drum, but this is necessary for several reasons. The model parameters were fitted with this system in action and therefore it seems sensible to include this in the optimization studies. Alternatively, both the reflux and distillate could be flow controlled at the expense of a path constraint to guarantee that the reflux drum does not run dry. However, path constraint problems are difficult to solve in comparison with unconstrained problems. Finally, any practical implementation on the plant would require some level control system on the reflux drum and there is no reason why the existing structure cannot be used. The time rate of change of the reflux drum level, M , is given by:

$$\frac{dM}{dt} = \frac{1}{k_R} \{V_1 - R - D\} \quad (3.20)$$

where k_R is a fitted parameter. Differential equations describing component changes in the reflux drum are identical to Eq.(3.18)

with $V_{out} = 0$. The distillate rate is then determined as:

$$D = D_o + k_T(M - M_o) \quad (3.21)$$

Where M_o and D_o are the initial reflux drum level and distillate rate respectively and k_T is a proportional controller gain.

Similarly, the reboiler drum (section 6) level is controlled by the bottoms flowrate.

Since the response of Q_6 to an increase in the fuel rate is not immediate, a first order lag is incorporated to account for the heat transfer delay. This gives:

$$\frac{dQ_6}{dt} = \frac{Q_R - Q_6}{\tau_R} \quad (3.22)$$

where Q_R is the heat to the reboiler and τ_R is a fitted parameter.

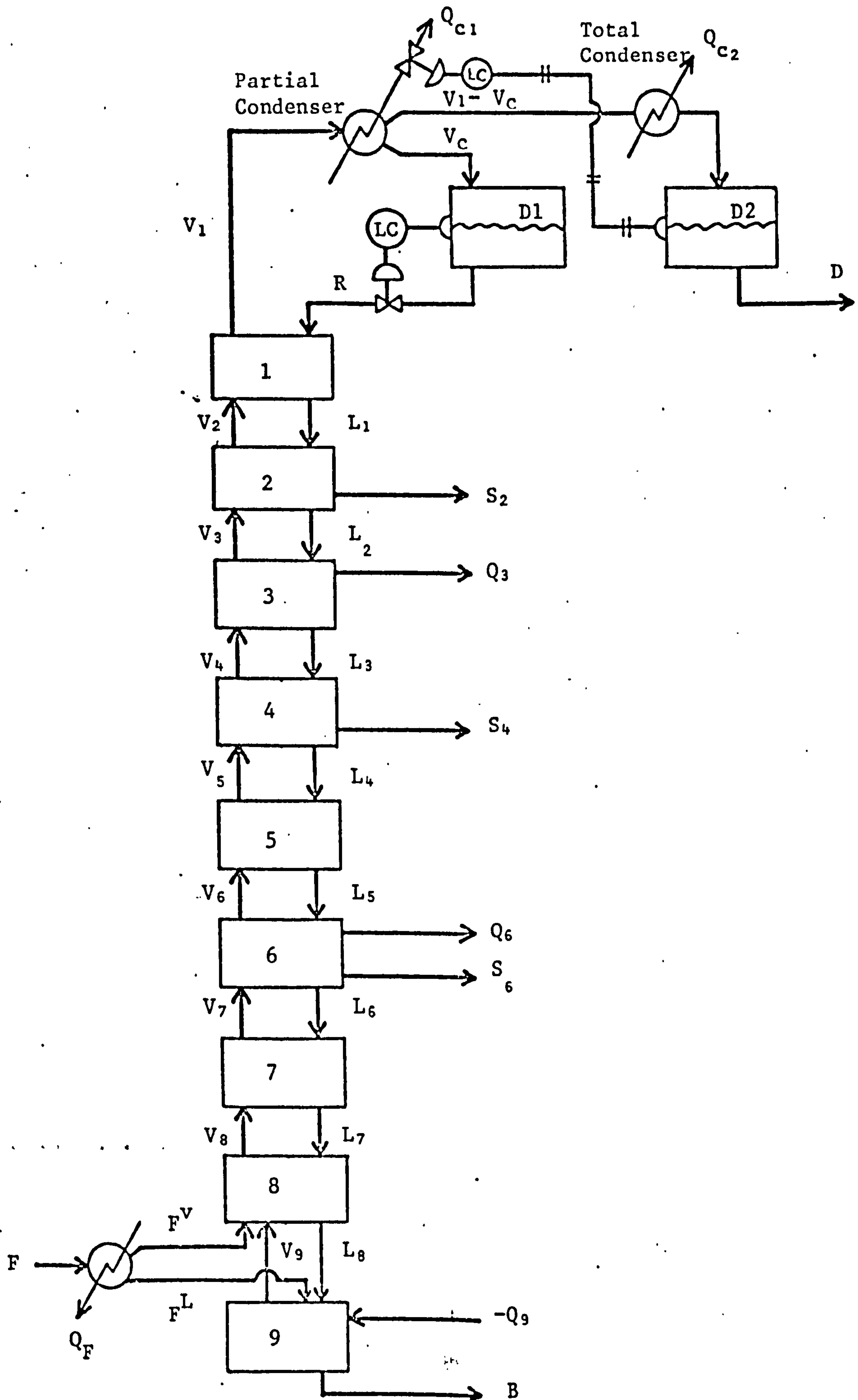
The order of the model is 28 and the total number of control variables is three: the reflux rate, R , the sidestream rate, S_2 , and the heat to the reboiler, $-Q_R$. For a transient response where these are specified together with feed temperature, composition and flowrates, right hand sides of Eq.(3.16)-(3.18) are evaluated working from the bottom of the column. In this manner, the term

$\frac{dV_{in}}{dt}$ in Eq.(3.16) and (3.17) is $\frac{dV_{out}}{dt}$ from the previous section, and $\frac{dV_{out}}{dt}$ in Eq.(3.17) comes from Eq.(3.16). The entering feed

is assumed to be at temperature, T_F , which determines the amount of feed vaporization and thus the feed liquid and vapour compositions. Product stream temperatures are predicted from linear combinations of the relevant section compositions.

3.1.3 The Main Column

As mentioned previously, the main column is structurally similar to the splitter except that there are five pseudo components and product streams instead of three. Fig. 3.4 illustrates

Figure 3.4 The Main Column

the main column sections. The describing differential equations for each section are identical to Eq.(3.16)-(3.18) but with Eq.(3.18) representing four components.

Note that the overheads system consists of two drums and two condensers: one partial and one total. The level of the first drum is controlled by the reflux while the cooling rate to the partial condenser governs the second drum level. It may be argued that considerable structure is specified and thus the optimal control is restricted within the confines of this structure. Relaxation of the overheads system structure is undertaken in section 3.1.4.

The main column model is represented by 62 ordinary differential equations and is controlled by 7 variables: D , S_2 , S_4 , S_6 , Q_3 , Q_6 , ϕ , where ϕ is the fraction of the total feed that is vaporized. The bottoms section heating rate, $-Q_9$, is nominally the stripping steam heat load which is held constant and the bottoms flowrate is used to control the level in section 9.

3.1.4 Main Column Model Reduction

Consider the main column illustrated in Fig. 3.4. The overheads systems, consisting of two drums, implies some control structure through the two level controllers. The role of drum D2 in optimal control calculations can be questioned. Its holdup is large in comparison with drum D1 or column sections and therefore only serves as a long lag for the entering flows and compositions. Furthermore, this sluggish response is transmitted firstly to drum D1 through the drum D2 level controller coupled to the partial condenser, and in turn to the entire column via the reflux flow. A restructuring of the overheads control system to effect faster

system responses would be beneficial.

A proposed modification to the overheads structure is shown in Fig. 3.5(a). The distillate rate, D , is now used to control the level in drum D2 while the condensed vapour feed, V_c , to drum D1 is free to control flow. Cooling requirements are no greater in this case since the entire overheads vapour is still eventually condensed. Note that the sluggish response has been isolated to drum D2 with no feedback to other parts of the system. In fact, because drum D2 is now a self-contained single-input-single-output system, it can be eliminated from the optimal control calculations. All column dynamics will be independent of D and the control of stream $(V_1 - V_c)$ specifications is consistent with plant objectives. Such a system is illustrated in Fig. 3.5(b). This has the advantages of faster response times without loss of flexibility in the control structure, and a reduction in the number of state variables. If the distillate rate, D , in Fig. 3.5(a) and associated compositions are necessary, these can be found by simply subjecting the optimal response of the vapour product, D , in Fig. 3.5(b) to the appropriate lags. For these reasons, the reduced overheads system depicted in Fig. 3.5(b) will be utilized.

Since the model differential equations are solved at each iteration during the optimization, any computing time reduction realized on a single transient response will be magnified as the optimization proceeds. A model will now be developed that closely resembles the presented BP model but has a lower model order. Assume that instantaneous holdups are proportional to the exit liquid flowrates (Rademaker et al., 1975) and vapour holdups are negligible. Thus:

Figure 3.5(a) Modified Overheads System

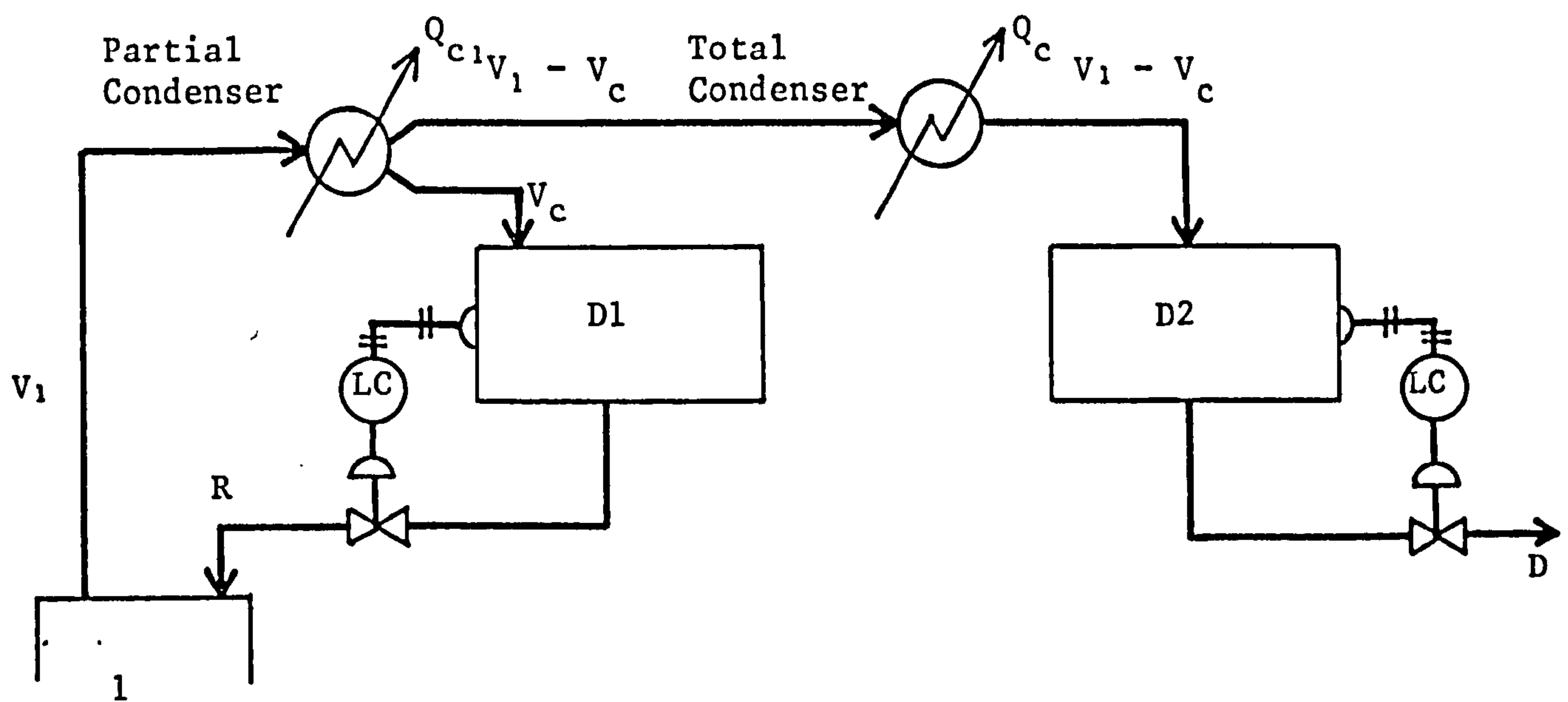
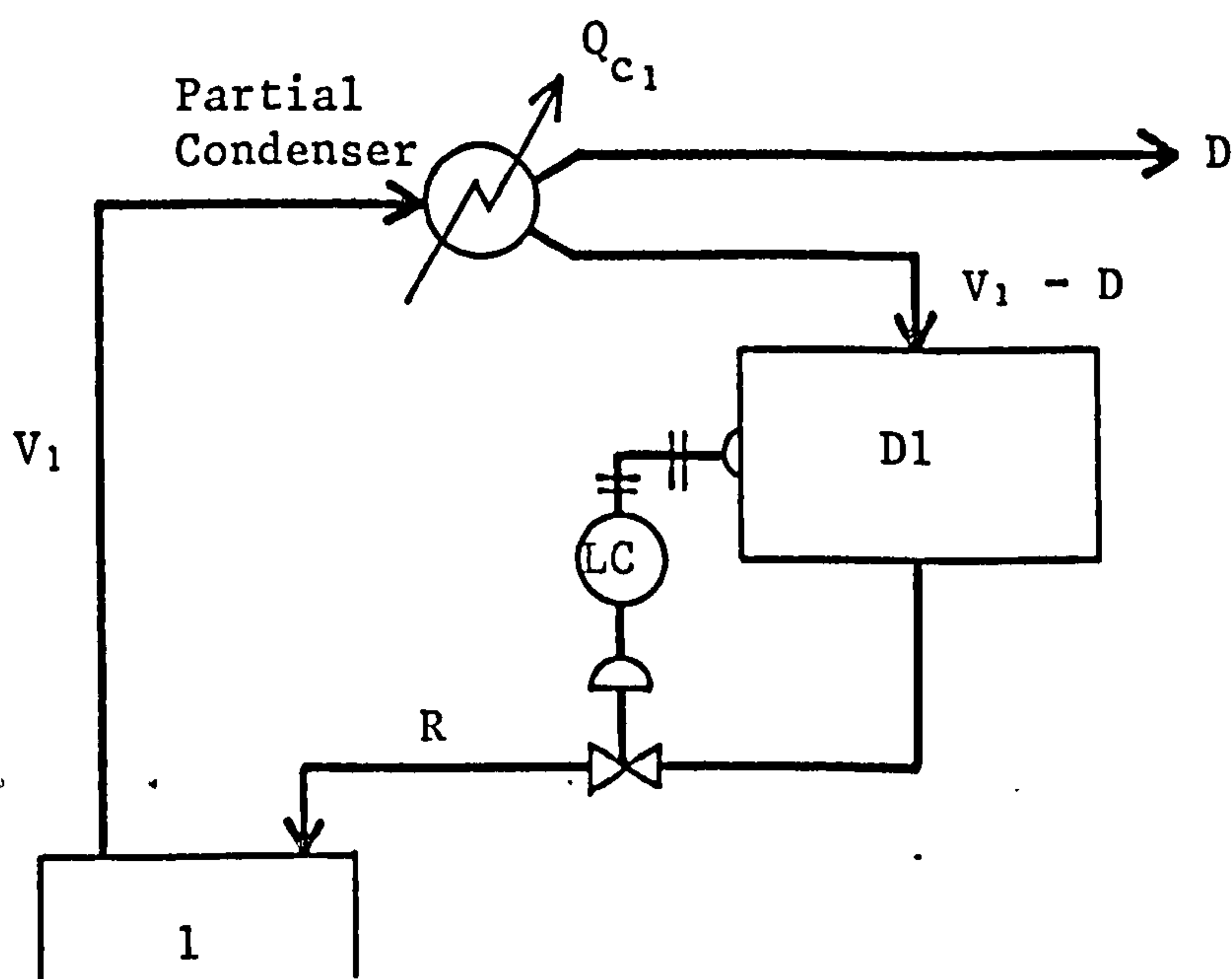


Figure 3.5(b) Modified Overheads System for Optimal Control



$$H = H_0 + k_1 L_{out} \quad (3.23)$$

where H_0 is the section holdup at the initial conditions. The time rate of change of mass and energy in a column section are:

$$\frac{dH}{dt} = V_{in} - V_{out} + L_{in} - L_{out} \quad (3.24)$$

$$\frac{d(He_{out})}{dt} = V_{in}E_{in} - V_{out}E_{out} + L_{in}e_{in} - L_{out}e_{out} - Q_{out} \quad (3.25)$$

where E and e are enthalpies of vapour and liquid respectively.

Assume:

- a) liquid and vapour have the same constant specific heat
- b) latent heat of vaporization, λ , is constant
- c) a constant temperature difference exists between the top and bottom of a section.

These assumptions were utilized in the development of the original model for which:

$$E_{out} - e_{in} = \lambda \quad (3.26)$$

$$E_{in} - E_{out} = e_{out} - e_{in} = \Delta e \text{ (constant)} \quad (3.27)$$

Relationships given by Eq.(3.26) and (3.27) are based on assumptions (a), (b), and (c) which are somewhat restrictive. One may argue that little more is lost if the enthalpy of the leaving liquid, e_{out} , is confined to be constant. From Eq.(3.26) and (3.27), all enthalpies are then constant, and Eq.(3.25) can be rewritten as:

$$\frac{dH}{dt} = \frac{1}{e_{out}} \{ V_{in}E_{in} - V_{out}E_{out} + L_{in}e_{in} - L_{out}e_{out} - Q_{out} \} \quad (3.28)$$

Define:

$$k = \frac{\lambda}{\lambda - \Delta e} \quad (3.29)$$

Equating (3.24) and (3.28) and solving for V_{out} using Eq.(3.29) yields:

$$V_{out} = kV_{in} - (k - 1)L_{in} - \frac{kQ_{out}}{\lambda} \quad (3.30)$$

Substituting H from Eq.(3.23) in Eq.(3.24) gives:

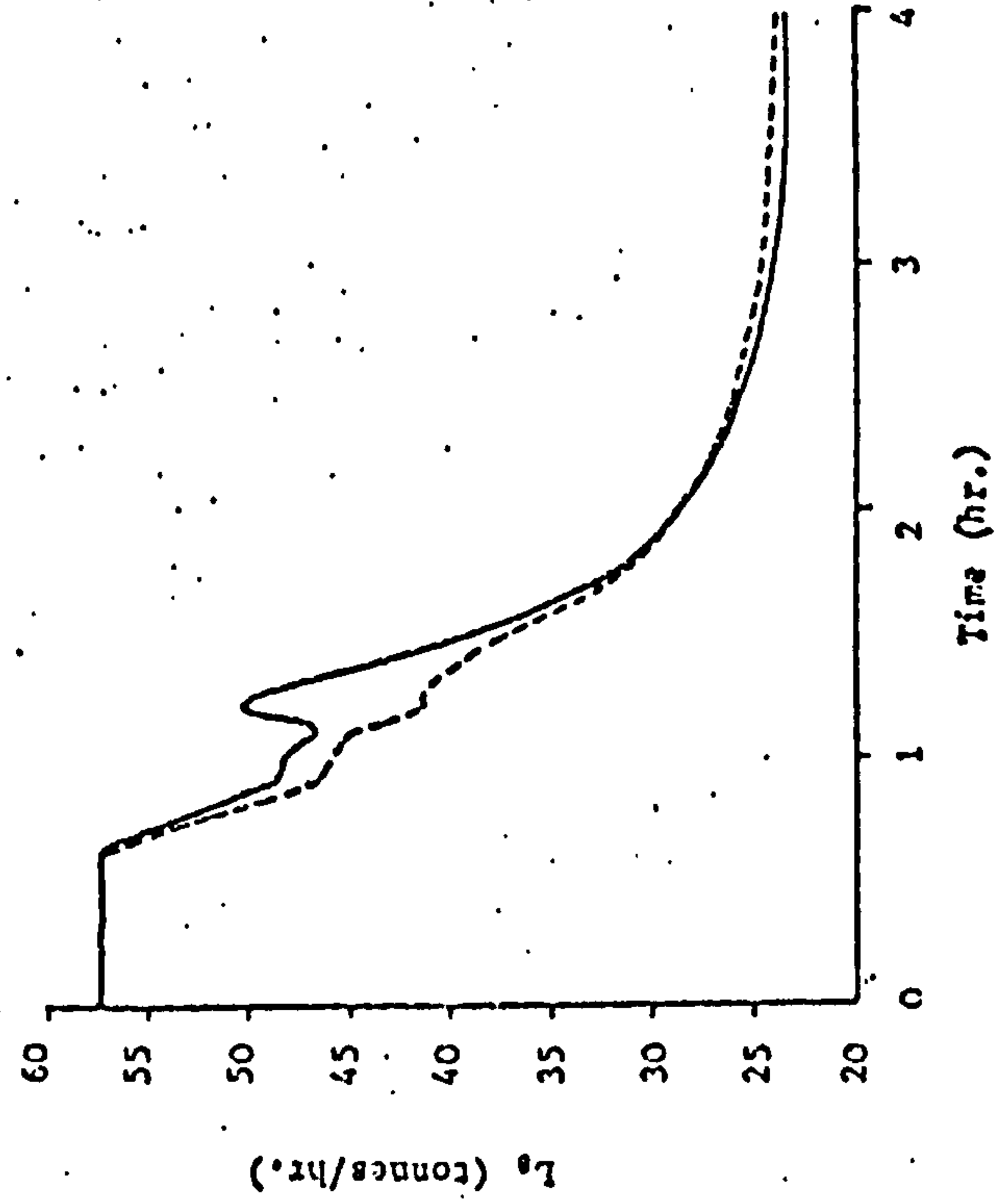
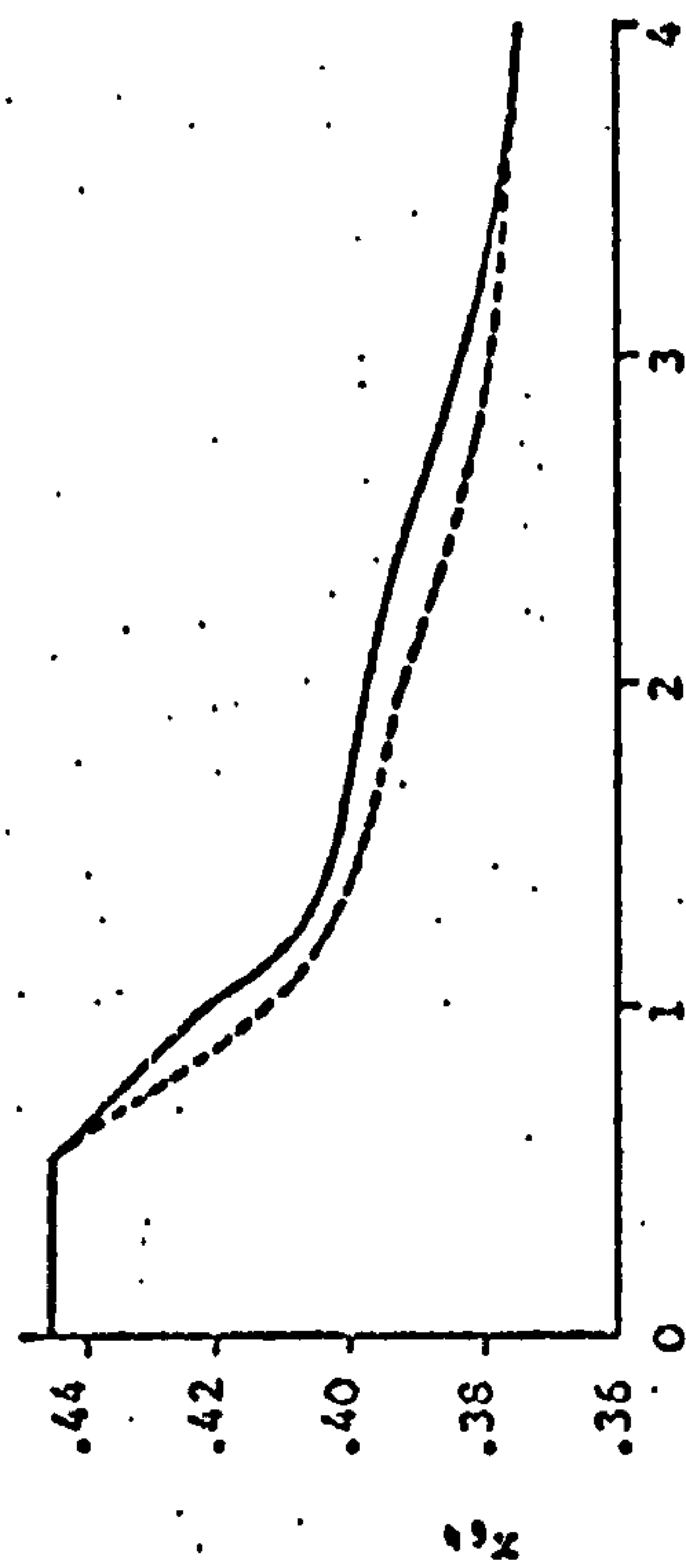
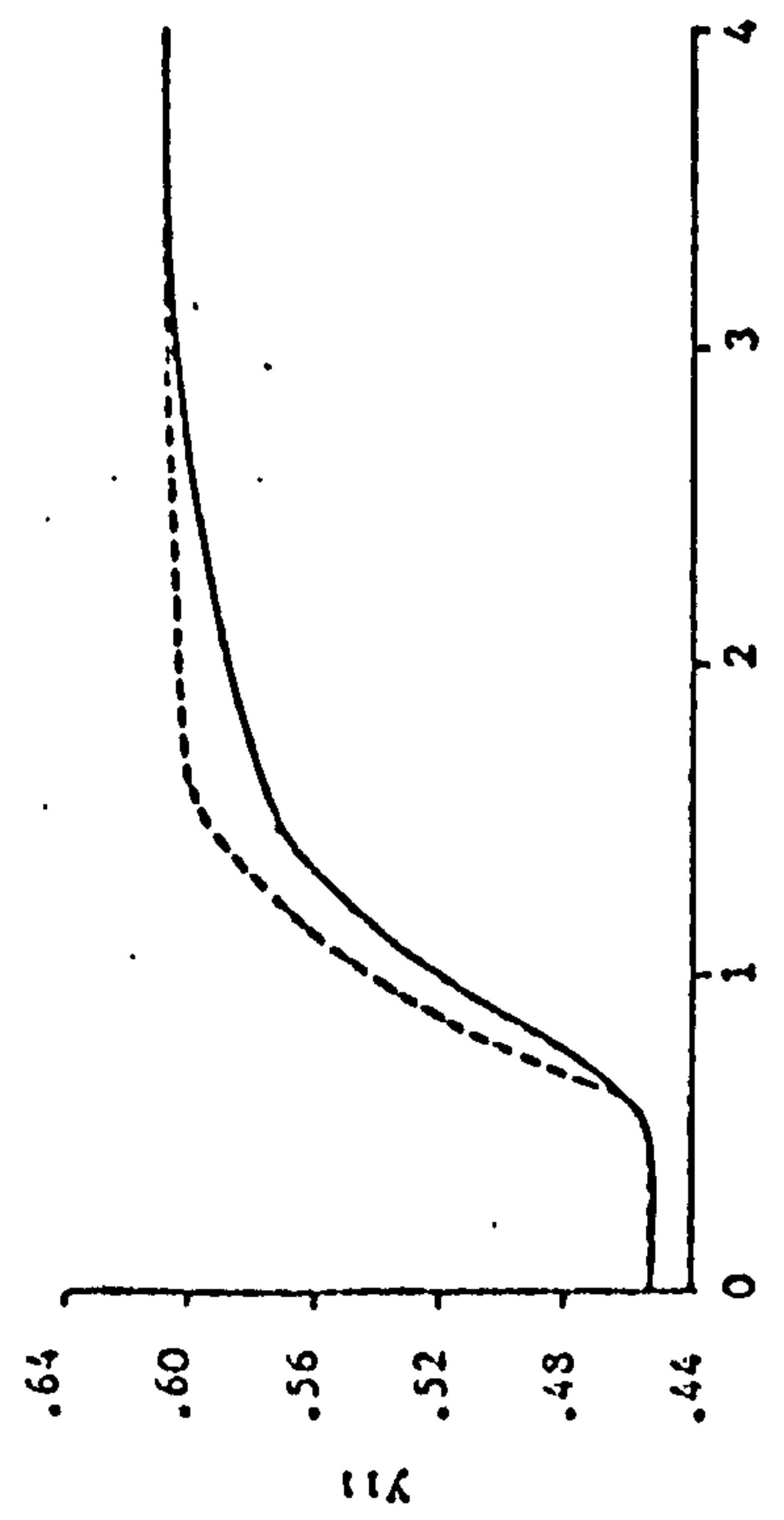
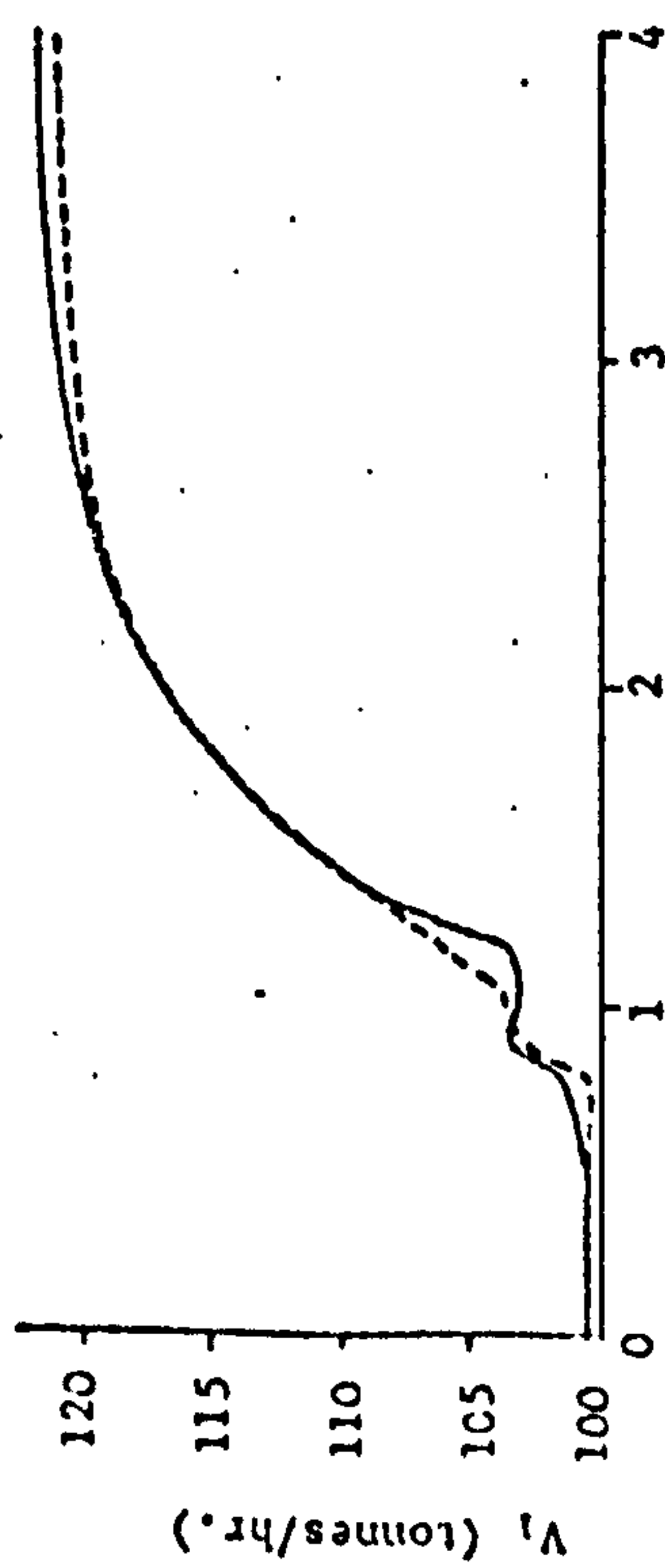
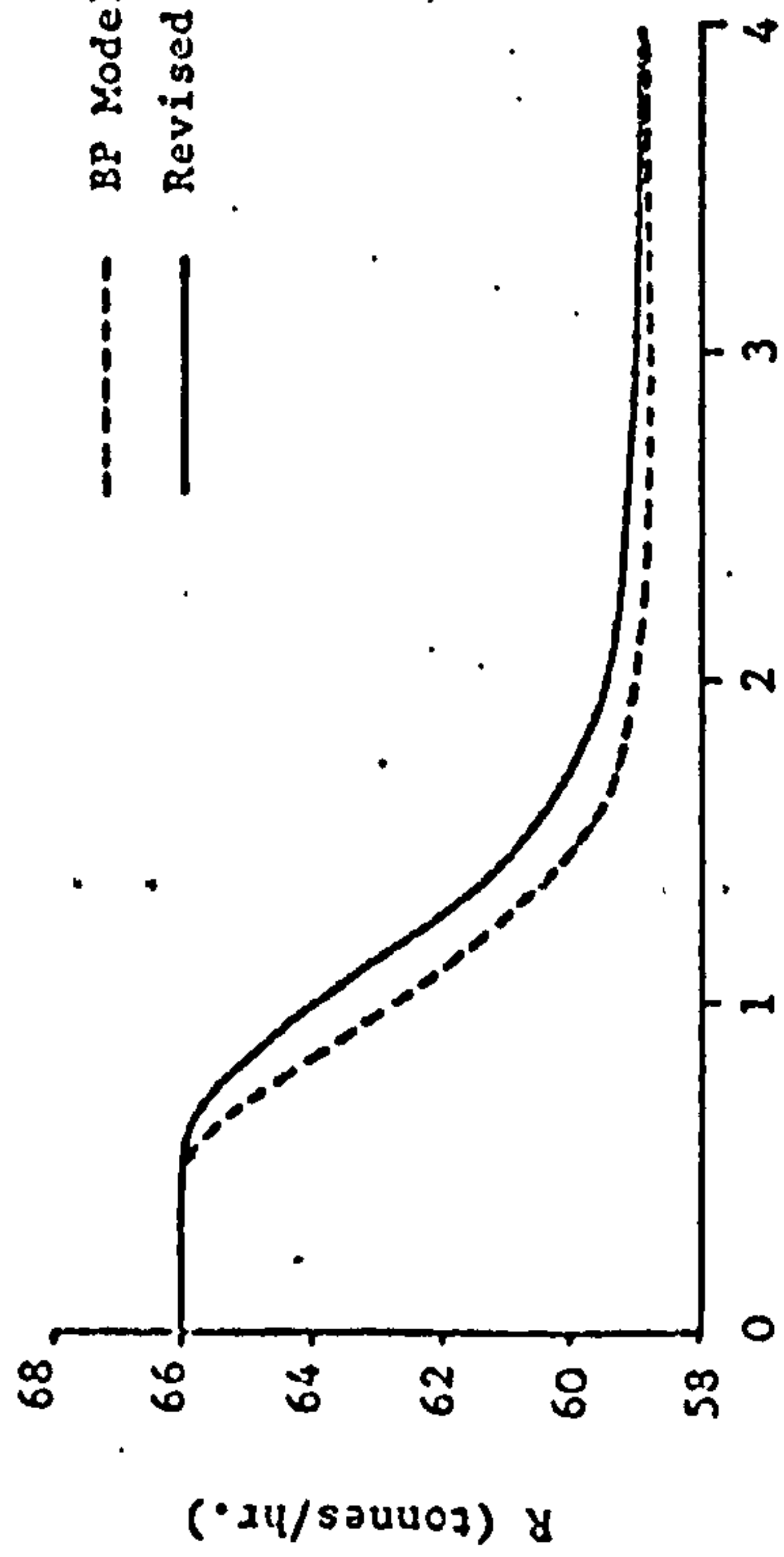
$$\frac{dL_{out}}{dt} = \frac{1}{k_1} \{V_{in} - V_{out} + L_{in} - L_{out}\} \quad (3.31)$$

Comparison of Eq.(3.30) and (3.31) to Eq.(3.16) and (3.17) reveals striking similarities between the two hydraulic models. Note that steady state solutions will be identical and in the dynamic case, $k_1 \approx \tau_H$. However, a transient response would be simpler to calculate for the modified model in that for each section, a differential equation has been replaced by an algebraic one. This suggests that if the models compare in a dynamic sense, implementation of the modified model would lead to some computational savings.

Simulations of a feed composition changeover were performed for the two models with the same control trajectories. For both models, the variable holdup method, which will be discussed in section 3.2.3, was used in the integration. Figure 3.6 illustrates some representative responses. The hydraulic responses for the modified model tend to be slightly more sluggish which cause slower composition responses. This could be overcome by tuning k_1 in Eq. (3.31). The only discrepancy in trends was the failure of the modified model to agree with the inverse response of the second section, second component composition predicted by the original model. However, in absolute terms, even this difference is within the accuracy of the identification experiments. Therefore, the modified hydraulic model will be adopted, with $k_1 = \tau_H$. Together with the simplification

Figure 3.6 Main Column Model Comparison

- - - BP Model
 — Revised Model



in the overheads system, this reduces the dimensionality of the main column model from 62 to 49.

3.2 Profit Objective Functions For Feed Changeover Problems

The objective function is central to optimal control calculations. A set of optimal controls is only as good as the performance index which should be chosen to represent plant objectives. Also, the objective function should reflect model accuracy; one which requires painstaking calculation should not be used in conjunction with a "cheap and dirty" model. For the crude changeover problem, controls must be determined to move steady state operation from one set of product specifications to another. It is assumed that the given initial and final steady states are optimal with respect to profit for the corresponding feed. Several types of objectives can then be envisaged for the changeover:

- a) minimize the changeover time
- b) minimize the off-specification product during the changeover
- c) maximize profit (minimize cost) during the changeover period.

For this application, the object is to realize a profit by producing on-specification product and thus it was decided to consider only objective function types (b) and (c). Type (b) will be discussed in section 3.3.

Consider a changeover from feed A to feed B over time t_o to t_f . Separate storage is available for each product corresponding to each crude. A profit type objective function has the form:

$$\begin{aligned}
 I = & \sum_{i=1}^{np} \left(Y_i^A \int_{t_o}^{t_f} r_i P_i dt + Y_i^B \int_{t_o}^{t_f} (1 - r_i) P_i dt \right) - \sum_{j=1}^{nh} \int_{t_o}^{t_f} C_j Q_j dt \\
 & + \{V_H(t_f) - V_H(t_o)\} - \int_{t_o}^{t_f} C_F F dt
 \end{aligned} \tag{3.32}$$

where:

- n_p is the number of product streams
- n_h is the total number of heat inputs and outputs
- P_i is the flowrate of the i th product stream
- r_i is the fraction of the i th product stream stored as product corresponding to feed A
- Q_j is the heat input of the j th heating (cooling) stream
- C_j is the cost of heating (cooling) the j th stream
- V_H is the value of the system holdup
- F is the feed rate to the column
- C_F is the cost of feed
- Y_i^A, Y_i^B are the unit values of the i th product stream stored as product corresponding to feed A and B respectively

The unit product stream values are functions of mole fractions of components in associated storage tanks. For example:

$$Y_i^A = f(x_{i1}^A, x_{i2}^A, x_{i3}^A, \dots x_{i,ncmp}^A) \quad (3.33)$$

where $ncmp$ is the number of components and x_{ij}^A , the mole fraction of the j th component in storage tank associated with the i th product and feed A, is given by:

$$x_{ij}^A = \frac{\int_{t_0}^{t_f} r_i P_i x_{ij} dt}{\int_{t_0}^{t_f} r_i P_i dt} \quad (3.34)$$

where x_{ij} is the mole fraction of the j th component in the i th product stream.

The optimal control routine is concerned with changes in the objective function for different control strategies. Every control

strategy will move the column from one steady state to another and since the holdups are uniquely defined by the liquid hydraulics the holdup change will be constant for a given crude change. Consequently, the fourth term in Eq.(3.32) can be discarded without affecting the optimal control policy. Using the same logic, the feed cost represented by the fifth term can also be dropped, and thus Eq.(3.32) reduces to:

$$I = \sum_{i=1}^{np} \{Y_i^A \int_{t_0}^{t_f} r_i P_i dt + Y_i^B \int_{t_0}^{t_f} (1 - r_i) P_i dt\} - \sum_{j=1}^{nh} \left\{ \int_{t_0}^{t_f} C_j Q_j dt \right\} \quad (3.35)$$

Note that the ratio-integral term in Eq.(3.34) does not fall into the class of objective functions denoted by Eq.(2.2). Recently Farhadpour and Gibilaro (1975) examined ratio integral objective functions of the form:

$$I = \frac{\int_{t_0}^{t_f} f_i(x, u, t) dt}{\int_{t_0}^{t_f} f_m(x, u, t) dt} \quad (3.36)$$

In an attempt to cast them as:

$$I = \int_{t_0}^{t_f} f_o(x, u, t) dt \quad (3.37)$$

This involved the addition of three new state variables given by:

$$\dot{x}_i = f_i \quad ; \quad x_i(0) = 0 \quad (3.38)$$

$$\dot{x}_m = f_m \quad ; \quad x_m(0) = 0 \quad (3.39)$$

and

$$\dot{x}_0 = f_0 = \frac{f_i x_m - f_m x_i}{x_m^2} ; x_0(0) = 0 \quad (3.40)$$

After considerable mathematical manipulation and discussion of continuity problems, the necessary conditions of optimality are derived. Such complications arise simply because the "standard" objective function denoted by Eq.(3.37) does not allow the possibility of functions of the final state as Eq.(2.2) does. If this were the case, then Eq.(3.36) would become:

$$I = \frac{x_i(t_f)}{x_m(t_f)} \quad (3.41)$$

where x_i and x_m are given by Eq.(3.38) and (3.39) respectively. The development of the necessary conditions now follows standard theory without undue complication.

In order to express Eq.(3.32) in the form of Eq.(3.41) using Eq.(3.33) and (3.34) an additional $2(np)(ncmp)$ state variables are required. For the main column model this would involve 50 extra differential equations, thus substantially increasing the model dimension. Simplifications are therefore sought which facilitate evaluation of total product value without significantly affecting the model order.

3.2.1 Marginal Values

One approach would be to ensure that f in Eq.(3.33) is linear with respect to composition. Several researchers (Sawargari et al., 1971; Rinjdsorp and Maarveld, 1969) in distillation control have used marginal values to determine product stream value. The unit value of the i th product stream, stored as feed A product, is given by:

$$y_i^A = v_i^A + \sum_{j=1}^{ncmp} M_{ij}^A (x_{ij}^A - x_{ij}^{A,*}) \quad (3.42)$$

where:

- V_i^A is the base unit value of the i th feed A product
 M_{ij}^A is the marginal value of the i th feed A product
 with respect to the j th component
 x_{ij}^A is the mole fraction of the j th component in the
 i th feed A product
 x_{ij}^{A*} is the reference mole fraction of the j th component
 in the i th feed A product

In this work, the models have been designed so that the interest in a product stream is centred on a key component and other components are assumed to have no influence on the product value. Hence, Eq.(3.42) becomes:

$$Y_i^A = V_i^A + M_i^A(x_i^A - x_i^{A*}) \quad (3.43)$$

where x_i^A is now the mole fraction of key component in the i th feed A product. Substituting Y_i from Eq.(3.43) and using Eq.(3.34) Eq.(3.35) becomes:

$$\begin{aligned} I = & \sum_{i=1}^{np} \left\{ \int_{t_0}^{t_f} [V_i^A + M_i^A (x_i - x_i^{A*})] r_i P_i dt + \int_{t_0}^{t_f} [V_i^B + M_i^B (x_i - x_i^{B*})] \right. \\ & \left. (1 - r_i) P_i dt \right\} - \sum_{j=1}^{nh} \left\{ \int_{t_0}^{t_f} C_j Q_j dt \right\} \\ = & \int_{t_0}^{t_f} \left\{ \sum_{j=1}^{np} P_i \left([V_i^A + M_i^A (x_i - x_i^{A*})] r_i + [V_i^B + M_i^B (x_i - x_i^{B*})] \right. \right. \\ & \left. \left. (1 - r_i) \right) - \sum_{j=1}^{nh} C_j Q_j \right\} dt \quad (3.44) \end{aligned}$$

which is in the form Eq.(2.2) without any additional state variables.

Note that there is one set of base unit values, marginal values, and reference concentrations for each product associated with each feed.

Sometimes, marginal value data is available from the linear program used to generate the optimum steady state conditions for each feed. However since the non-linear dynamic models are not consistent with the linear program models, in a steady state sense, the optimal steady state conditions predicted by the two models would differ and thus present a serious drawback for the implementation of the optimal controls. The same observation could be expected for any set of arbitrary marginal value data. Therefore, it is necessary to seek sets of base values, marginal values, and reference concentrations that guarantee consistency between the optimum steady state obtained from the dynamic models and known operating conditions.

For any feed, the steady state objective function can be deduced from Eq.(3.44) as:

$$I_{ss} = \sum_{i=1}^{np} P_i \{V_i + M_i(x_i - x_i^*)\} - \sum_{j=1}^{nh} C_j Q_j \quad (3.45)$$

If all product stream flowrates, except one, all heating rates, except one, and reflux flow, R , are known, the column will be completely specified. The undetermined product and heating rates are given by mass and energy balances respectively. Assume that all product specifications and flowrates do not lie upon operating constraints. Then the gradients of the optimal steady state objective function, $\hat{I}_{ss}$, with respect to the selected variables will be zero. These gradients are given by:

$$\begin{aligned} \frac{\partial \hat{I}_{ss}}{\partial P_i} = & \sum_{k=1}^{np} V_k \frac{\partial P_k}{\partial P_i} + \sum_{k=1}^{np} \frac{\partial P_k}{\partial P_i} M_k (\hat{x}_k - x_k^*) + \sum_{k=1}^{np} P_k M_k \frac{\partial \hat{x}_k}{\partial P_i} \\ & - \sum_{j=1}^{nh} C_j \frac{\partial Q_j}{\partial P_i} \quad i = 1, 2 \dots np - 1 \end{aligned} \quad (3.46)$$

$$\begin{aligned} \frac{\partial \hat{I}_{ss}}{\partial R} = & \sum_{k=1}^{np} \frac{\partial P_k}{\partial R} M_k (\hat{x}_k - x_k^*) + \sum_{k=1}^{np} P_k M_k \frac{\partial \hat{x}_k}{\partial R} - \sum_{j=1}^{nh} C_j \frac{\partial Q_j}{\partial R} \end{aligned} \quad (3.47)$$

$$\begin{aligned} \frac{\partial \hat{I}_{ss}}{\partial Q_j} = & \sum_{k=1}^{np} \frac{\partial P_k}{\partial Q_j} M_k (\hat{x}_k - x_k^*) + \sum_{k=1}^{np} P_k M_k \frac{\partial \hat{x}_k}{\partial Q_j} - \sum_{k=1}^{nh} C_k \frac{\partial Q_k}{\partial Q_j} \\ & j = 1, 2 \dots nh - 1 \end{aligned} \quad (3.48)$$

In order to simplify these expressions, set:

$$x_i^* = \hat{x}_i \quad (3.49)$$

That is, the reference concentration for each product stream has been equated to the steady state optimal concentration. This together with the fact that the partial derivative of one independent variable with respect to another is zero reduces Eq.(3.46)-(3.48) to:

$$V_i - V_{np} + \sum_{k=1}^{np} P_k M_k \frac{\partial \hat{x}_k}{\partial P_i} - C_{nh} \frac{\partial Q_{nh}}{\partial P_i} = 0 ; i = 1, 2 \dots np - 1 \quad (3.50)$$

$$\sum_{k=1}^{np} P_k M_k \frac{\partial \hat{x}_k}{\partial R} - C_{nh} \frac{\partial Q_{nh}}{\partial R} = 0 \quad (3.51)$$

$$C_{nh} - C_j + \sum_{k=1}^{np} P_k M_k \frac{\partial \hat{x}}{\partial Q_j} = 0 ; j = 1, 2, \dots, nh - 1 \quad (3.52)$$

If the partial derivatives in Eq.(3.50)-(3.52) could be estimated from steady state data, a set of $np + nh - 1$ linear equations in $2np + nh$ unknowns ($V_i, M_i; i = 1, 2, \dots, np; C_j, j = 1, 2, \dots, nh$) results leaving $np + 1$ degrees of freedom. In other words, if $np + 1$ of the base values, marginal values or heating costs could be specified, the remainder could be derived from the solution of Eq.(3.50)-(3.52) in order to ensure consistency between the model and plant operating conditions. A similar analysis can be performed for the constrained case.

To demonstrate this approach, consider the splitter model as depicted in Fig.3.3. The cooling water rate to the condenser is fixed from plant data and does not enter into calculation. In the steady state, the specification of the distillate, reflux and sidestream rates leads to a section by section solution where Q_c and B are determined from balances. A digital computer program (SSSP) was written to accomplish this. The right hand sides of Eq.(3.16) and (3.17) were set to zero and by working down the column V_{in} and L_{out} for each section were evaluated. Using Eq.(3.19), the time invariant solution of Eq.(3.18) (12 non-linear equations, 12 unknowns) was obtained with a secant method (Gragg and Stewart, 1976).

For given feed conditions (feed A), the steady state concentrations were calculated to a tolerance of 10^{-8} . This yielded $\hat{x}_1 = .5700014$, $\hat{x}_2 = .5021790$, $\hat{x}_3 = .4686623$. A finite difference analysis was then performed by slightly perturbing the initial independent variables and recalculating the steady state. Values of the partial derivatives are shown in Table 3.1. The amount of

TABLE 3.1 FINITE DIFFERENCE ANALYSIS FOR FEED A

Splitter Operating Conditions

F = 65 tonnes/hr

D = 16 tonnes/hr

R = 65 tonnes/hr

S₂ = 30 tonnes/hr

Feed temperature = 127.5 °C

Feed composition:

 $z_{F1} = .30$ $z_{F2} = .45$ $z_{F3} = .25$

Perturbations:

 $\Delta D = .1$ tonnes/hr $\Delta R = .5$ tonnes/hr $\Delta S_2 = .5$ tonnes/hrPartial Derivatives

Dependent Variable	x ₁	x ₂	x ₃	Q ₆ thermies/hr.*
Independent Variable				
D	-.010546	.0015852	.0077074	-43.290
R	.0006817	-.0005469	.0019163	-87.068
S ₂	-.0034110	-.0006701	.0058591	22.164

* Calorific Value of Fuel: $\cdot 10^4$ Thermies/tonne

perturbation for each variable was determined by preliminary analysis to yield a compromise between round-off error and size of perturbation.

Four of the required values must be given a priori in order to evaluate the other three. British Petroleum supplied accurate estimates of the product base values as well as the cost of fuel. These were: $V_1 = 600$ \$/tonne, $V_2 = 580$ \$/tonne, $V_3 = 570$ \$/tonne, $C_1 = .035$ \$/thermie. Substitution into Eq. (3.50) and (3.51) ($n_h = 1$, therefore Eq.(3.52) not included) resulted in a linear system of three equations in three unknowns. This was solved to yield: $M_1 = 187.17$, $M_2 = 51.74$, $M_3 = 4.31$. These results are physically realistic since they reflect that similar increases in product specification are more valuable closer to the top of the column.

In order to test the marginal values, steady state objective functions were evaluated from Eq.(3.45) near the optimum and the results are shown in Table 3.2. The objective function values in this table appear to be large because the cost of feed is not accounted for. Note that $\hat{I}_{ss}$ is indeed optimal and for large changes in the independent variables, as denoted by the last entry, objective function changes are significant.

3.2.2 Optimal Stream Fractioning Policies

The solution of the optimal control problem with profit objective function given by Eq.(3.44) would involve the choice of thenp dimensional vector of storage fraction parameters, $r(t)$, as well as the controls. For distillation problems, this effectively doubles the number of optimization variables and

TABLE 3.2 SPLITTER STEADY STATE OBJECTIVE FUNCTION VALUES NEAR
OPTIMUM CONDITIONS

Optimum Conditions: D = 16.0 Tonnes/hr.
 (Feed A) R = 65.0 Tonnes/hr.
 $S_2 = 30.0$ Tonnes/hr.
 $\hat{I}_{ss} = 37719.79970$ \$/hr.

Value of Perturbed Variable	I_{ss}
D = 15.90	37719.77881
D = 16.10	37719.77963
R = 64.50	37719.77343
R = 65.50	37719.79968
R = 66.00	37719.77410
$S_2 = 29.90$	37719.79871
$S_2 = 30.10$	37719.79939
D = 13.00	37700.70793

thus an incentive is provided to examine the problem structure for possibilities of size reduction. A first approach may be to confine $r(t)$ to be either zero or one; each product stream must be fed entirely into a single storage tank at any one time. However, this requires formulation of special switching times for $r(t)$ which would necessitate alterations to the standard OPCON package. It therefore may be more instructive to examine the problem directly.

Eq.(3.44) can be rewritten as:

$$I = \int_{t_0}^{t_f} \left[\sum_{i=1}^{np} \{r_i W_i^A + (1 - r_i) W_i^B\} - \sum_{j=1}^{nh} C_j Q_j \right] dt \quad (3.53)$$

where W_i^A and W_i^B are instantaneous values of the i th product stream sent to tank A and B respectively. Since $r(t)$ does not appear in the describing state differential equations, $W_i^A(t)$ and $W_i^B(t)$ can be determined independently of $r(t)$. For any control policy, $u(t)$, Eq.(3.53) can be minimized with respect to $r(t)$. Since this process applies for any admissible control trajectory, the optimal control problem can be solved separately if the optimal stream fractioning policy were known. Because of the linearity of r in Eq.(3.53), simple a priori laws can be derived for stream fractioning policies. Consider the following optimal control problem where only $r(t)$ is treated as the control:

Choose: $r_i(t)$; $i = 1, 2, \dots, np$

To minimize: $-x(t_f)$

Subject to: $\dot{x} = \sum_{i=1}^{np} \{r_i W_i^A + (1 - r_i) W_i^B\} - \sum_{j=1}^{nh} C_j Q_j$;
 $x(0) = 0$ (3.54)

$$0 \leq r_i(t) \leq 1 \quad ; \quad i = 1, 2, \dots, np \quad (3.55)$$

The control, $r(t)$, appears linearly in the state differential equation. It is well known (Bryson and Ho, 1969) that the solution to this type of problem is bang-bang in the control. Therefore, it is optimal to store each product stream at any one time entirely in tank A or tank B. However, the problem still remains of specifying when to switch each stream from one tank to another. This can be solved by examining the gradient of the objective function with respect to the switch time. This gradient for t_i , the switching time from tank A to tank B for the i th product stream, together with the adjoint system is given by: (see Eq.(2.22), (2.23))

$$\dot{\lambda} = 0 \quad ; \quad \lambda(t) = \lambda(t_f) = -1 \quad (3.56)$$

$$\frac{\partial I}{\partial t_i} = \lambda(W_i^A - W_i^B) = W_i^B - W_i^A \quad (3.57)$$

At the optimum, the gradient will be zero which leads to the switching condition:

$$W_i^A = W_i^B \quad \text{at} \quad t = t_i \quad (3.58)$$

The same condition prevails for a switch from tank B to tank A.

Therefore, the optimal stream fractioning policy can be stated as:

$$r_i = 1, \quad W_i^A \geq W_i^B \quad ; \quad i = 1, 2, \dots, np \quad (3.59)$$

$$r_i = 0, \quad W_i^A < W_i^B \quad ; \quad i = 1, 2, \dots, mp \quad (3.60)$$

When $W_i^A = W_i^B$ the objective function value is independent of fractioning policy and an arbitrary choice of r_i can be made. Here, r_i is chosen to equal 1.

The optimal control problem can now be solved with the objective function evaluated according to switching conditions given by Eq.(3.59) and (3.60). Using this method, the product stream fractioning parameters have been eliminated from the set of optimization variables at virtually no computational expense. This could not have been accomplished without employing marginal values. In other situations, the additional state variables needed to specify x_{ij} in Eq.(3.34) would effect interaction between optimal product stream fractioning and optimal control policies.

3.2.3 Consistency of Models for Profit Objective Functions

The profit objective function was developed assuming that the column inventory change was constant in moving operation between two specified steady states, no matter what changeover control policy was used. This is indeed the case on the plant because the steady state section holdups are uniquely determined by the operating conditions. It must be ensured that the models themselves possess this property or else the optimization will discriminate between various control policies in order to create more profitable holdup changes (i.e. less final holdup, more product). The lower order model presented in section 3.1.4 was developed to be holdup consistent. Now the original model, given by Eq.(3.16)-(3.19) will be analyzed. The time rate of change of section holdup is:

$$\frac{dH}{dt} = L_{in} + V_{in} - L_{out} - V_{out} \quad , \quad H(0) = H_o \quad (3.61)$$

Define:

$$L'_{in} = L_{out} + V_{out} - V_{in} \quad (3.62)$$

The describing differential equation for L'_{in} can be derived from

Eq.(3.17) as:

$$\frac{dL'_{in}}{dt} = \frac{1}{\tau_H} \{L_{in} - L_{out} + V_{in} - V_{out}\} \quad (3.63)$$

Comparing Eq.(3.61) and (3.63), it is obvious that:

$$\Delta H = \tau_H \Delta L'_{in} \quad (3.64)$$

In the steady state, from Eq.(3.62):

$$L_{in} = L'_{in} \quad (3.65)$$

Since the inlet flowrate to each section, L_{in} , is uniquely defined in the steady state, so is L'_{in} via Eq.(3.65). For a change from one steady state to another, the holdup can then be uniquely determined from Eq.(3.64). A similar analysis for the reflux drum leads to:

$$\Delta H_R = k_R \Delta M \quad (3.66)$$

where ΔH_R is the reflux drum holdup change which is unique for changes between given steady states. Therefore, the entire system holdup change is independent of changeover control policy.

The same argument can be applied to any component inventory. The model should not allow the creation of valuable component at the expense of cheaper component. For a changeover between t_o and t_f , the holdup change of the j th component in a column section is given by:

$$\int_{t_o}^{t_f} \frac{d(Hx_j)}{dt} dt = \int_{(Hx_j)_o}^{(Hx_j)_f} d(Hx_j) = (Hx_j)_f - (Hx_j)_o = K \quad (3.67)$$

where K is a constant.

Eq.(3.56) can also be written as:

$$\int_{t_o}^{t_f} d(Hx_j) = \int_{t_o}^{t_f} x_j dH + \int_{t_o}^{t_f} H dx_j = K \quad (3.68)$$

Although the sum of the two terms in Eq.(3.68) is always a constant which is independent of the changeover control trajectory, in general neither term by itself is constant. In Eq.(3.18), which describes the time varying j th component concentration, a constant holdup value, say H^* , was assumed. This simplification was considered unlikely to significantly affect the composition trajectories. Eq.(3.68) then becomes:

$$\begin{aligned} \int_{t_o}^{t_f} d(Hx_j) &= \int_{t_o}^{t_f} x_j dH + H^* \int_{t_o}^{t_f} dx_j = \int_{t_o}^{t_f} x_j dH + H^*(x_j(t_f) \\ &\quad - x_j(t_o)) \end{aligned} \quad (3.69)$$

The first term on the right hand side of Eq.(3.69) will be control trajectory dependent since holdup changes are accounted for in the hydraulic model. However, the second term is fixed for a given changeover and thus these types of models are subject to variations in component holdup changes for various control trajectories.

This problem can be circumvented by using a variable holdup for the integration of Eq.(3.18). The time varying holdup is readily available as demonstrated in the previous discussion concerning total mass inventory. From Eq.(3.63) and (3.64):

$$H = H_o + \tau_H \{L_{out} + V_{out} - V_{in} - (L_{out} + V_{out} - V_{in})_o\} \quad (3.70)$$

Similarly, for the reflux drum:

$$H_R = H_{R_0} + k_R \{ M - M_0 \} \quad (3.71)$$

During the integration, the time varying holdups can be determined using Eq.(3.70) and (3.71) and subsequently employed to evaluate the right hand side of Eq.(3.18).

In order to illustrate this property, an accurate trapezoidal integration was performed for both constant holdup (CH) and variable holdup (VH) splitter models for three arbitrary control trajectories during a feed changeover. A new state variable, H_T , was added to represent the middle component holdup in the system. Its dynamics are given by:

$$\frac{dH_T}{dt} = \sum_{i=1}^6 H_i x_{i2} + H_R x_{R2}, \quad H_T(0) = 0 \quad (3.72)$$

where x_{R2} is the middle component composition in the reflux drum. For both cases, the holdup values in Eq.(3.72) were calculated from Eq.(3.70) and (3.71). However, in model CH the initial holdup was used for the composition trajectories (i.e. $H = H^* = H_0$ in Eq. (3.18)), whereas the time varying holdup was employed for model VH. If final steady state control is applied for sufficient time at the end of the dynamic period, $H_T(t_f)$ should predict the total middle component inventory change for the changeover.

The results for these runs are shown in Table 3.3. Since operation is moved from one steady state to another, the component holdup change should be independent of control trajectory. From Table 3.3 it is clear that this is the case for model VH but not for CH. The changeover in this example was simply a feed temperature change. Where feed composition or flowrate changes

TABLE 3.3 COMPARISON OF MIDDLE COMPONENT INVENTORY CHANGE FOR
MODELS CH AND VH WITH VARIOUS CONTROL TRAJECTORIES

Feed Temperature Changeover

Control Trajectory	$H_T(t_f)$ (tonnes)	
	Model CH	Model VH
1	-.350	-.405
2	-.521	-.405
3	-.280	-.405

occur, even greater discrepancies than those demonstrated here can be expected. For this reason, model VH will be adopted to deal with profit objectives for the remainder of this work.

3.3 Objective Function Comparison

A consistent profit objective function has been formulated that ensures agreement between model and plant steady states. Properties of this objective function can now be investigated along with expected control trends that result from its application. An identical analysis can be performed for the squared set point deviation objective function which is given by:

$$I_{DSP} = \int_{t_0}^{t_f} \sum_{i=1}^{np} \{r_i (x_i - x_i^A)^2 + (1 - r_i) (x_i - x_i^B)^2\} dt \quad (3.73)$$

Here the stream fractioning parameters, r , are determined by the method outlined in section 3.2.2. Note that calculation of I_{DSP} simply requires knowledge of the optimal steady state operating conditions as opposed to the rather involved marginal value information necessitated by a profit objective function (I_p). Therefore, if employment of I_p and I_{DSP} yield similar control trends for changeover problems, the squared deviation from set point objective function could be used confidently.

From the changeover problem definition, both objective functions will effect a change in operation between two known steady states. However, each objective will manipulate the dynamics differently to meet its particular needs. For example, maximization of I_p may prolong the dynamic period in order to operate more profitably. The following question can then be

posed: Given the freedom to operate dynamically on a single feed, will minimization of either $(-I_p)$ or I_{DSP} exhibit preference to unsteady state operation over optimum steady state operation?

3.3.1 Comparison of Optimal Steady State and Dynamic Policies

The fact that periodic operation of chemical processes yields better objective function values than optimal steady state control was mathematically validated by Horn and Lin (1967). Various tests have been developed to determine conditions under which this occurs. These include the maximum principle test (Bailey and Horn, 1971), relaxed steady state analysis (Bailey and Horn, 1971), singular control test (Matsubara et al., 1975), and the π -test (Bittanti et al., 1973). For this work, the first and second order conditions originally formulated by Horn and Lin will be used. Consider a process given by:

$$\dot{x} = f(x, u, t) \quad (3.74)$$

Then the optimal control problem is formulated as (Horn and Lin, 1967):

Choose: $u(t)$

$$\text{To Minimize: } I = \int_0^{t_f} J(x, u, t) dt \quad (3.75)$$

$$\text{Subject to: } \dot{x} = f(x, u, t) \quad (3.76)$$

$$\dot{\lambda} = -f_x^T \lambda - J_x^T \quad (3.77)$$

$$x(t_f) = x(0) \quad (3.78)$$

$$\lambda(t_f) = \lambda(0) \quad (3.79)$$

Boundary condition (3.79) ensures that the process is periodic. The necessary and sufficient conditions for the minimization of

I are:

$$I_u = J_u + \lambda^T f_u = 0, \quad 0 \leq t \leq t_f \quad (3.80)$$

$$I_{uu} = J_{uu} + f_{uu}^T \lambda > 0, \quad 0 \leq t \leq t_f \quad (3.81)$$

Now consider the equivalent steady state problem:

Choose: u

To minimize: $J(x, u)$

Subject to: $f(x, u) = 0 \quad (3.82)$

By taking gradients with respect to the control, the following necessary and sufficient conditions for the minimization of J are found:

$$J_u - F_x^T f_x^{-1} f_u = 0 \quad (3.83)$$

$$\begin{aligned} J_{uu} - f_{uu}^T (f_x^{-1})^T J_x^T + [f_{xu}^T f_x^{-1} f_u + f_u^T (f_x^{-1})^T f_{ux}^T \\ - f_u^T (f_x^{-1})^T f_{xx}^T f_x^{-1} f_u] (f_x^{-1})^T J_x^T - f_u^T (f_x^{-1})^T J_{xu} \\ - J_{ux} f_x^{-1} f_u + f_u^T (f_x^{-1})^T J_{xx} f_x^{-1} f_u > 0 \end{aligned} \quad (3.84)$$

Suppose the optimal solution for the steady state problem is (x^*, u^*) . The application of u^* over the entire time period will now be examined in terms of dynamic optimality. By setting $x(0) = x^*$, the matrices, f_x^T and J_x^T , in Eq.(3.77) become time invariant and using Eq.(3.79), the adjoint vector, λ , is:

$$\lambda^T(t) = \lambda^{T*} = - J_x^T f_x^{-1}; \quad 0 \leq t \leq t_f \quad (3.85)$$

Substitution into Eq.(3.80) and (3.81) yields:

$$I_u = J_u - J_x^T f_x^{-1} f_u; \quad 0 \leq t \leq t_f \quad (3.86)$$

$$I_{uu} = J_{uu} - f_{uu}^T (f_x^{-1})^T J_x^T ; \quad 0 \leq t \leq t_f \quad (3.87)$$

Note that at the steady state optimum, the first order conditions for dynamic optimality, Eq.(3.86), are automatically satisfied by Eq.(3.83). However, the second order dynamic optimality conditions given by Eq.(3.87) represent only the first two terms of Eq.(3.84). One could therefore envisage situations where condition (3.84) is satisfied but I_{uu} in Eq.(3.87) would be less than zero. That is, the control which minimizes the steady state performance index maximizes the dynamic objective function.

These concepts are best illustrated through a simple scalar example. A single state, single control, linear/quadratic problem, in which parameters a , b , q , r are scalar constants, is given by:

$$\begin{aligned} \text{Choose:} & \quad u \\ \text{To Minimize:} & \quad I = \int_0^{t_f} (qx^2 + ru^2) dt \end{aligned} \quad (3.88)$$

$$\text{Subject to:} \quad \dot{x} = ax + bu \quad (3.89)$$

The equivalent steady state problem is:

$$\begin{aligned} \text{Choose:} & \quad u \\ \text{To Minimize:} & \quad J = qx^2 + ru^2 \end{aligned} \quad (3.90)$$

$$\text{Subject to:} \quad ax + bu = 0 \quad (3.91)$$

Eq.(3.91) can be used to eliminate x from Eq.(3.90) to give:

$$J = (q \frac{b^2}{a^2} + r)u^2 \quad (3.92)$$

The first and second order conditions for steady state optimality given by Eq.(3.83) and (3.84) become:

$$2(q \frac{b^2}{a^2} + r)u = 0 \quad (3.93)$$

$$2(q \frac{b^2}{a^2} + r) > 0 \quad (3.94)$$

From Eq.(3.87), any steady state control is dynamically optimal only if:

$$r > 0 \quad ; \quad 0 \leq t \leq t_f \quad (3.95)$$

The necessary condition, from Eq.(3.93), for steady state optimality is:

$$u = 0 \quad (3.96)$$

since $r = -q \frac{b^2}{a^2}$ results in the trivial case of a zero objective function for any control. Using Eq.(3.94), the sufficient conditions for optimal steady state control is:

$$r > -q \frac{b^2}{a^2} \quad (3.97)$$

For simplicity, consider only $q > 0$. Then two cases emerge:

- (i) $r > 0$: This satisfies condition (3.95) and (3.97).
Therefore the control which minimizes the steady state objective function also minimizes the dynamic performance index.
- (ii) $-q \frac{b^2}{a^2} < r < 0$: This satisfies condition (3.97) but violates (3.95) which means conditions at the steady state minimum correspond to a dynamic maximum.

Case (ii) is worthy of comment. The control, $u = 0$, is optimal in the steady state sense because, even though r is negative, any other control will increase the objective function through the influence on the state. For the dynamic situation, an infinite series of switches between $u = +\infty$ and $u = -\infty$ results in negatively infinite objective function as opposed to zero for application of

optimal steady state control. In fact, many finite sequences of switches exist that demonstrate improvement over constant zero control.

For the special case, $r = 0$, the second order conditions for dynamic optimality as given by Eq.(3.81) become:

$$I_{uu} = 0 \quad , \quad 0 < t < t_f \quad (3.98)$$

which denotes a saddle point. This occurs because the objective reflects only the state trajectory and not that of the control. Therefore, any control policy which yields the optimal state trajectory (i.e. series of infinite switches of any amplitude) is an optimal dynamic control. For practical purposes, only the optimal steady state control is of direct interest. However, note that $r = 0$ does represent the transition between minimizing and maximizing the dynamic objective function by application of optimal steady state control.

The two objective functions in question for distillation systems can now be examined. In terms of deviation from set point state variables for a single feed, Eq.(3.44) and (3.73) can be rewritten as:

$$I_P = \int_0^{t_f} \{ (x - x^*)^T R (x - x^*) + (x - x^*)^T P u + c^T u + d^T (x - x^*) \} dt \quad (3.99)$$

$$I_{DSP} = \int_0^{t_f} (x - x^*)^T Q (x - x^*) dt \quad (3.100)$$

The terms $(x - x^*)^T R (x - x^*)$ and $d^T (x - x^*)$ in Eq.(3.99) arise because the bottom product rate is a state rather than a control. For the relevant model equations given by Eq.(3.16)-(3.20), the

control variables appear linearly in the state differential equations (i.e. $f_{uu} = 0$). Therefore, with both I_P and I_{DSP} , Eq.(3.81) reduces to:

$$I_{P_{uu}} = I_{DSP_{uu}} = 0 \quad (3.101)$$

Eq.(3.101) indicates that optimal steady state controls cannot be guaranteed to be optimal in a dynamic sense. Clearly, for objective I_{DSP} no value lower than that obtained by using optimal steady state control can be found. However, infinite switching policies can be postulated that track the optimal state trajectories and thus account for a saddle point. In the same manner, the saddle point for $-I_P$ can be explained but the existence of dynamic policies which yield lower objective function values than that resulting from optimal steady state control cannot automatically be discounted. Some assurance can be obtained by examining the properties of objective function I_P' given by:

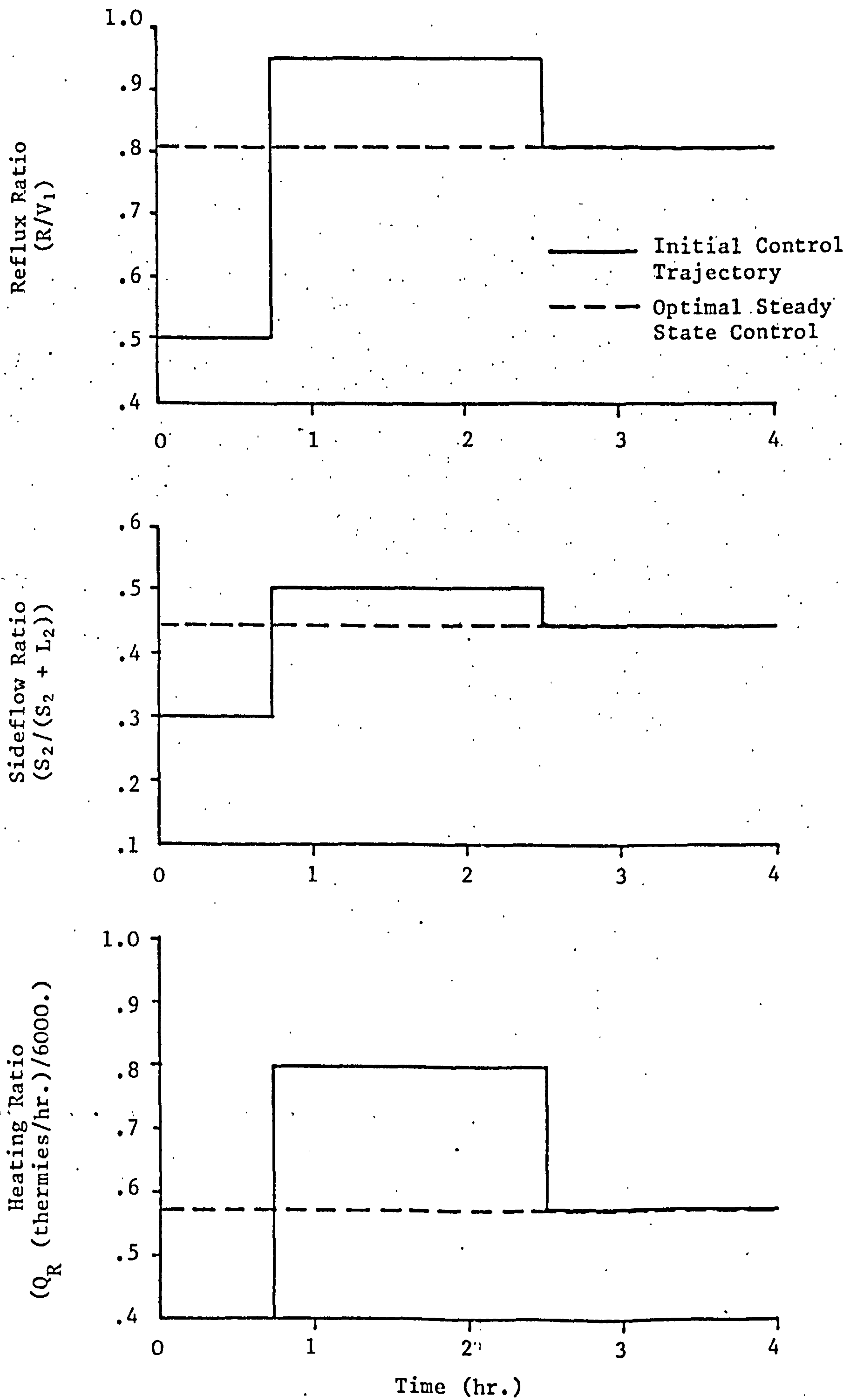
$$I_P' = \int_0^{t_f} \{ (x - x^*)^T R (x - x^*) + (x - x^*)^T P u + d^T (x - x^*) + c^T u + u^T E u \} dt \quad (3.102)$$

The steady state optimal control minimizes I_P' for $E > 0$, and maximizes I_P' for $E < 0$. The transition is represented by $E = 0$ or $I_P = I_P'$. (i.e. analogous to $r = 0$ in linear/quadratic example).

In order to confirm the suspicion that optimal steady state control is dynamically optimal for I_P , a series of tests were established for the splitter model. The column was initially at the optimal steady state conditions for feed A. For continued operation on feed A over a period of 4 hours, OPCON was given

freedom to choose control trajectories to minimise I_p . Optimal steady state control was implemented over the last 0.8 hours to guarantee attainment of the optimal steady state conditions at the final time. As suggested by Horn and Lin (1967), each of the controls were separately perturbed away from the optimal steady state level during the first 0.2 hours. In each case, OPCON re-established optimal steady state control in a few iterations, rather than promoting a cyclic operation. As a final test, the initial trajectory was chosen as shown in Fig. 3.7. By altering control levels and switching times, after 7 iterations, OPCON had forced the control trajectory to within one per cent of the optimal steady state control. Based on these results, it can be concluded that for objective function I_p , optimal steady state control represents a local dynamic optimum.

Throughout the analysis, the number of variables available for control in the dynamic and steady state cases have been assumed to be equal. This is not necessarily true for distillation applications. For example, for steady state purposes, one of the product flowrates becomes a state in order to satisfy the overall mass balance. In the dynamic problem, this flowrate may be utilized as a control at the expense of a final time constraint to ensure an overall holdup balance. Thus, the control space dimensionality of the dynamic problem exceeds that of the steady state equivalent and it is clear, as demonstrated by Matsubara et al. (1975), that dynamic policies exist which yield higher efficiencies than optimal steady state control. However, since the models in this work possess implied structure through the overheads and bottoms level control systems and since the feed rate changes are fixed, the number of free control variables are

Figure 3.7 Steady State Control Test For Splitter

are the same for both cases.

3.3.2 Feed Changeover Comparison

It is now apparent that neither I_p or I_{DSP} will lead to a preference of unsteady state operation over optimal steady state control. When operation changes between two optimal steady states, both objective functions should tend to shorten the dynamic period in order to reach steady state operation. I_p will perform this task with a compromise on fuel whereas I_{DSP} will attempt to minimize the off-specification product. In order to examine the effect on control trends, OPCON was run for a splitter feed changeover using both objective functions. Data for the combined feed composition and temperature changeover is shown in Table 3.4. The total changeover time was taken as 3 hours with final steady state control applied for the final 0.8 hours.

Values of the two objective functions for the solution to the two optimizations are shown in Table 3.5. Here, the profit objective value is less feed cost which was determined by evaluating feed as bottom product. Note that OPCON driven by I_{DSP} gives almost the same value of profit as using I_p for the objective function. This indicates that profit forms a very flat optimum showing large insensitivity to control trajectory. More sensitivity is achieved with a squared deviation from set point objective as demonstrated in the last column of Table 3.5. From these results, it is clear that I_{DSP} can be used to replace I_p for feed changeover problems.

3.3.3 Constraint Representation

Formulation of feed changeover problems involves three types

TABLE 3.4 DATA FOR DYNAMIC OBJECTIVE FUNCTION COMPARISON

FEED	A	B
Entrance Time (hrs)	0	0.5
Feed Rate (tonnes/hr)	65	65
Feed Temperature ($^{\circ}\text{C}$)	127.5	117.5
Feed Composition:		
z_{F1}	.30	.25
z_{F2}	.45	.40
z_{F3}	.25	.35
Fuel Cost (\$ /thermie)	.035	.035
Base Product Values		
V_1	600	600
V_2	580	580
V_3	570	570
Optimal Set Points:		
x_1^*	.5700	.5836
x_2^*	.5022	.4587
x_3^*	.4687	.5620
Marginal Values:		
M_1	187.17	228.88
M_2	51.74	59.31
M_3	4.31	9.74

TABLE 3.5 DYNAMIC OBJECTIVE FUNCTION COMPARISON

Driving Objective Function	Objective Value	
	(+I _P)-Feed Cost (\$)	I _{DSP}
-I _P	1318	2.57 x 10 ⁻³
I _{DSP}	1309	1.53 x 10 ⁻³

of constraints:

- a) The control flowrates and heating rates are bounded by minimum and maximum values represented by physical plant limits.
- b) The state at the end of the changeover period must correspond to the optimal steady state of the new feed.
- c) During the entire changeover period, internal liquid and vapour rates must remain positive.

The optimal control package deals naturally with constraint type (a). Type (b) is of the form:

$$x_i(t_f) - x_i^* = 0 \quad ; \quad i = 1, 2, 3, \dots, n \quad (3.103)$$

where x_i is the i th state variable (either flow or composition) and x_i^* is its optimal final steady state value. In some cases, where the number of state variables appearing in the objective function (I_{DSP}) is at least equal to the number of degrees of freedom for the system it is not necessary to impose this constraint. Minimization of the performance index will then be consistent with reaching the new desired steady state, providing a sufficient time period for control is allowed. For this reason, the final steady state constraint will be applied only to the main column. Rather than formulating n final time constraints, it is possible to specify a single end time constraint:

$$\sum_{i=1}^n (x_i(t_f) - x_i^*)^2 = 0 \quad (3.104)$$

In general, each step in the optimization will require several costly evaluations of differential equation solutions to ensure feasibility of Eq.(3.104). Alternatively, since the final steady state control vector, u^* , is known, its application for approximately

three system time constants at the end of the changeover period will automatically satisfy Eq.(3.103). One drawback is that simulations must be determined over longer periods of time but this is more than offset by savings realized from elimination of the final time constraint.

The approach is consistent with plant operating policy because, after the changeover, final steady state control is implemented to maintain optimal specifications for the new feed. Also since the objective is to minimize deviations from the optimal setpoints, if sufficient changeover time is allowed in OPCON, final steady state control can be expected to emerge even before its specified time of application. If this is the case, the resulting contribution to the objective function during the extended end time should be negligible.

Constraint type (c) are path constraints which also require several evaluations of the differential equations at each step of the optimization. Negative liquid and vapour rates result from large drawoff flows which tend to run the column dry. In order to circumvent these path constraints, upper bounds on the liquid drawoff rates could be established that would never allow dry column conditions to occur. For the debutanizer and splitter, this type of approach will be adopted. However, for the main column, where internal liquid flowrates can vary much more than for the other two columns, this representation could inhibit the flexibility of OPCON; sometimes at high internal liquid flowrates, it may be advantageous to remove an unusually high amount of material. Therefore, control constraints are sought for the main column that reflect the time varying nature of the column conditions.

Consider a column section in which the total exit liquid flowrate, L_{out} , is divided into a liquid drawoff, S , and a liquid rate, L_c , to the section below. Thus:

$$L_{out} = L_c + S \quad (3.105)$$

The control used to adjust the drawoff rate is not S directly but the ratio, R_S , defined by:

$$R_S = \frac{S}{L_{out}} \quad (3.106)$$

A lower bound on R_S is zero corresponding to no drawoff rate, whereas $R_S = 1$ indicates total drawoff with no liquid flow to the next section. Clearly, the latter situation is undesirable and realistic upper bounds on R_S can be obtained from plant operating data. The drawoff rate is determined as:

$$S = R_S L_{out} \quad (3.107)$$

Note that for a constant value of R_S , the drawoff rate is proportional to the total liquid flowrate leaving the section. In a similar manner for the overheads system illustrated in Figure 3.5(b), the control variable, R_D , is defined as:

$$R_D = D/V_1 \quad (3.108)$$

Thus, these types of control variables eliminate the necessity of path constraints without severely limiting the flexibility of the remaining control system. Although the plant is controlled by direct drawoffs, these can be easily obtained from any simulation using Eq.(3.107).

In summary, by careful examination of the system structure, feed changeover problems with bounded controls, final time and path constraints have been transformed into problems with simple

bounded controls. Computational savings from such simplifications are expected to be large.

CHAPTER 4 - OPTIMAL CONTROL STUDIES FOR DEBUTANIZER AND SPLITTER

4.1 Introduction

This chapter deals with the optimal control and implementation aspects of crude changeover problems for the splitter and debutanizer. Crude changeovers are represented by a combination of feed upsets and specification changes. Past optimal control studies of distillation units for regulatory and servo problems have been largely restricted to binary columns with linear dynamics and quadratic performance index (LQP) in order to capitalize on the quick feedback solutions through the Riccati equation. However, control sensitivity to the choice of the performance index weighting matrices and region of linearization has been demonstrated by several researchers (Rafal and Stevens, 1968; Hu and Ramirez, 1972; Chan and Talbot, 1975). Controllers derived by McGinnis and Wood (1974) using the same approach for a reduced order model experienced difficulties due to model inaccuracies.

Apart from the LQP, few other optimal control problems for binary columns have been attempted. For the special case of a zero control cost and instantaneous set-point objective, a bang-bang control law results. Although some experimental studies validate good performance of this controller (Brosilow and Handley, 1968; Merluzzi and Brosilow, 1972), Oakley and Edgar (1975) found that it led to excessive switching as the steady state was approached. Open loop simulation studies by Pollard and Sargent (1970a) utilized a non-linear model in conjunction with an integral profit objective.

In order to circumvent difficulties associated with local linearization, the approach adopted here is to perform the optimal control on the non-linear models, followed by an investigation into the optimal responses. By observation of common trends apparent in the responses, an underlying control philosophy is sought, and implementation that incorporate this philosophy is discussed. In this manner, a control structure that is valid over the entire dynamic period emerges.

In reality, the debutanizer and splitter are stepping stones for the main column studies. However, in their own right, they do represent interesting problems in distillation control. The simple control laws that are developed for the debutanizer changeover can be used in any binary system for similar applications. Apart from minimum variance regulator analysis by Jacobs and Dyer (1975) on a ternary system, no other optimal control calculations have been undertaken for a column with more than two product streams. Therefore, the full optimal control of the splitter provides insight into the control of a column with a sidestream drawoff.

4.2 The Debutanizer

The debutanizer is the simplest of the three columns and thus provides a logical starting point for the optimal control studies. Since there is no intermediate storage between the main column top product stream and the debutanizer, a feed changeover for this unit occurs shortly after a crude column distillate specification change. This interaction seemingly violates the basic premise of independent control system synthesis for each of the units. However, the debutanizer optimal

control analysis will be based on step composition changes and this is consistent with good control of a main column feed changeover.

Good control performance of the debutanizer is interpreted as fast product specification changeover with a minimum of off-specification material. This can be easily formulated as the squared deviation from set point type objective function discussed in section 3.3.1. Sometimes, owing to a changing economic environment, it is desirable to move product qualities to a new steady state at the same feed conditions. Conversely, in the face of feed upsets it may be beneficial to maintain product specifications. For all these objectives, knowledge of final steady state control supplies two advantages: information as to reachability of the final specifications within the confines of the control limits as well as a good initial estimate for calculation of the optimal control. Therefore, before any dynamic optimization of the debutanizer is attempted, the steady state behaviour will be investigated.

4.2.1 Steady State Analysis

In the steady state, for given feed conditions, product stream temperatures are uniquely defined by the concentration of heavy component in tops, y_T , and light component in the bottoms, x_B . These, in turn, are determined by controls through the two quadratic equations:

$$a_T y_T^2 + b_T y_T + c_T = 0 \quad (4.1)$$

$$a_B x_B^2 + b_B x_B + c_B = 0 \quad (4.2)$$

where coefficients a_T , b_T , c_T , a_B , b_B , c_B are non-linear

functions of controls (reflux, R , and fuel rate, Q), and the feed conditions. For specified top and bottom temperatures, T_T , T_B , the controls R , Q are sought in order to satisfy Eq.(4.1) and (4.2). A digital computer program (DBSS) was written that accepted column feed conditions and product temperature as input, and calculated controls using a Newton method.

A set of typical results from DBSS is shown in Figure 4.1. Reflux and fuel rates were found for various values of feed flowrate, F , feed temperature, T_F , and feed concentration of light component, z_F , in order to maintain set points, x_B^* and y_T^* . The linear relationship between feed flowrate and controls is demonstrated in Figures 4.1(a) and 4.1(b). Note that Figure 4.1(a)

illustrates the insensitivity of the required steady state reflux to the feed temperature, in this range of interest. The difference between the broken and solid lines at $z_F = 0.39$ shows the largest variation for the two extremes of feed temperature, whereas at $z_F = 0.31$ this difference is indistinguishable.

Conversely, the steady state fuel rate exhibits a high sensitivity to feed temperature as shown in Figure 4.1(c).

4.2.2 Dynamic Optimal Control

The dynamic optimization was performed using an objective function of the form:

$$I = \int_0^{t_f} \{ (T_T - T_T^*)^2 + (T_B - T_B^*)^2 \} dt \quad (4.3)$$

where T_T^* , T_B^* are temperature set points for the top and bottom product streams respectively. Equal weightings have been assumed for stream temperature deviations and this is consistent with

Figure 4.1 Debutanizer Steady State Controls to Maintain Setpoints

$$x_B^* = .300$$

$$y_T^* = .300$$

Figure 4.1(a)

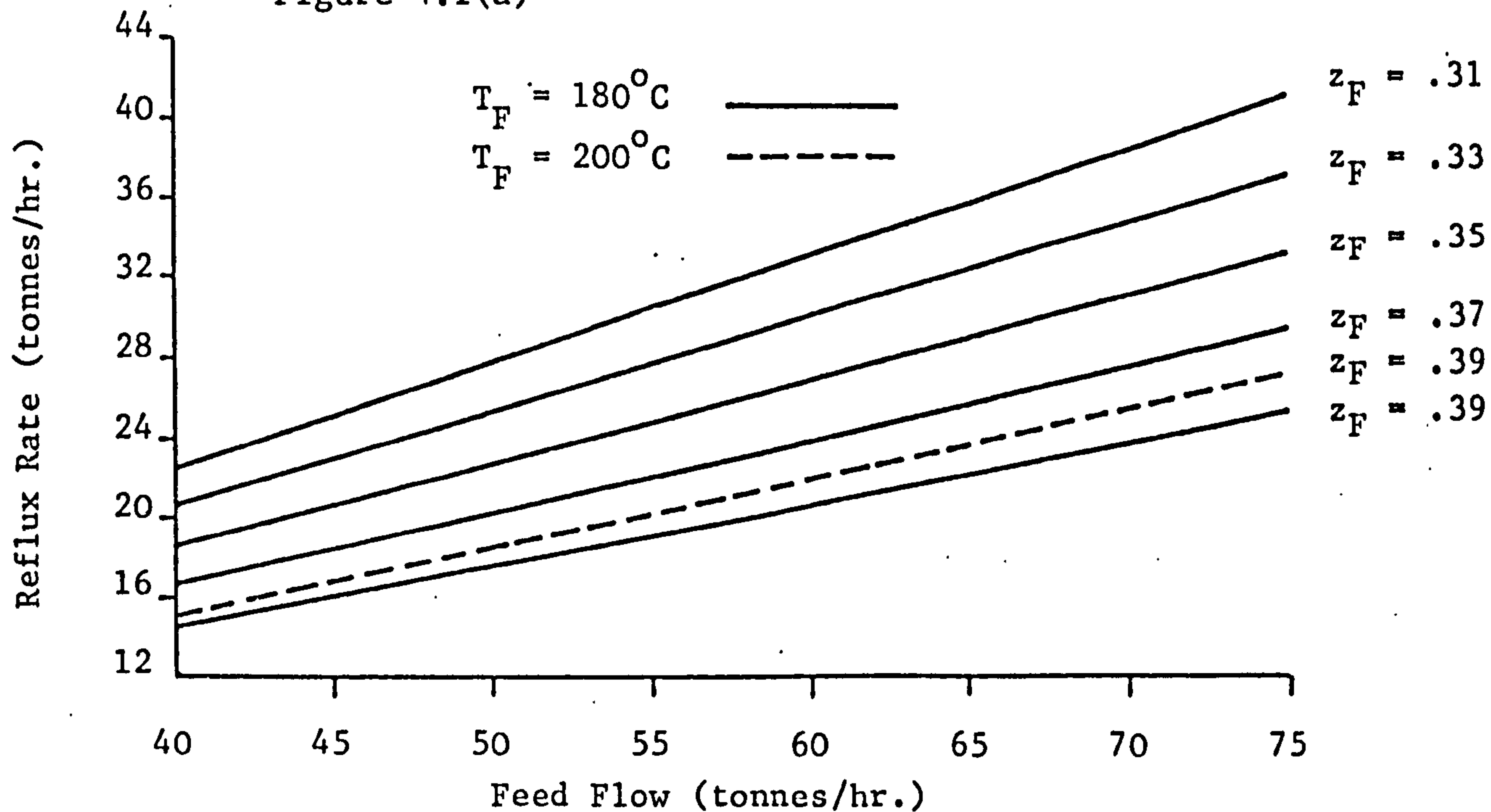


Figure 4.1(b)

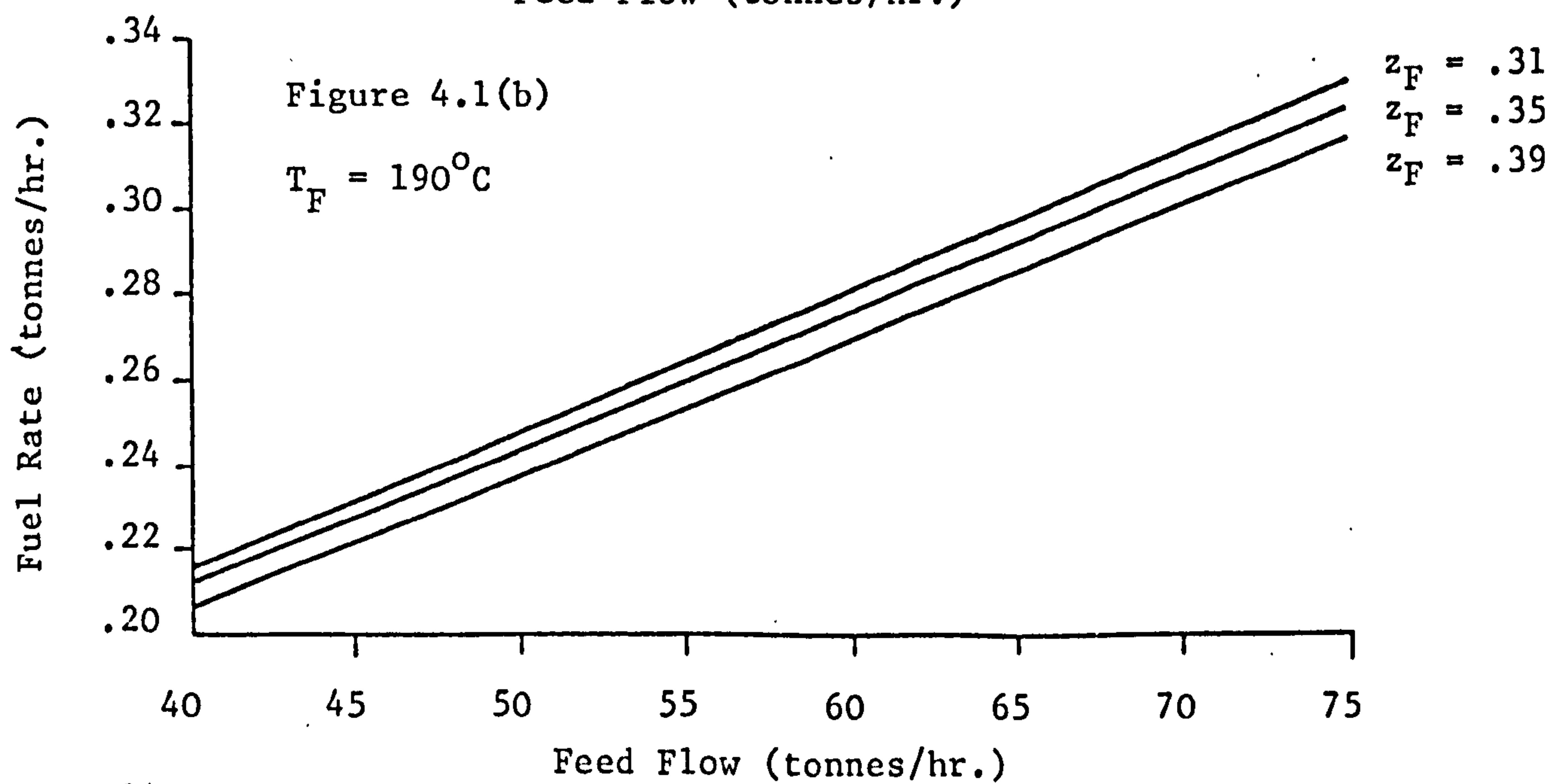
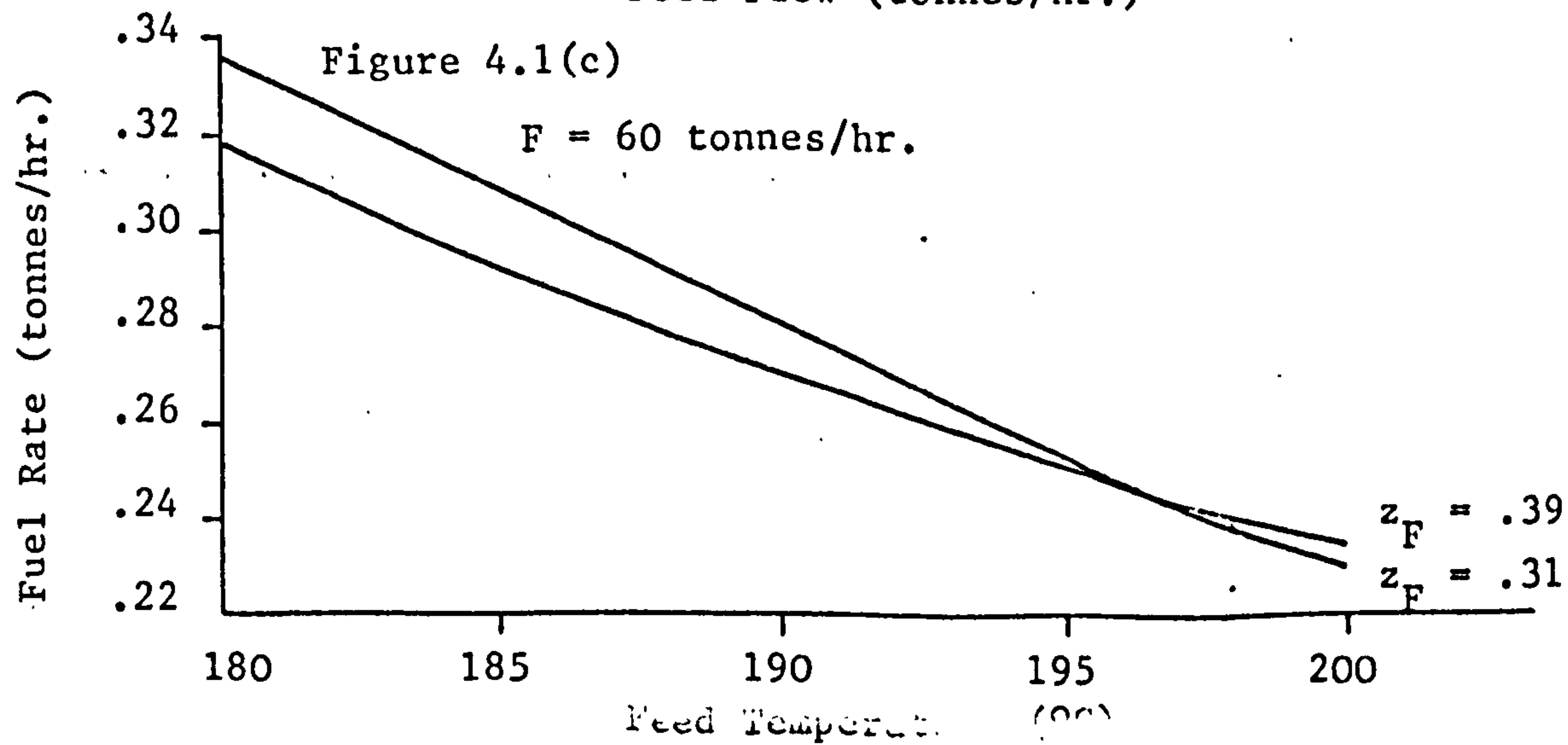


Figure 4.1(c)



plant operating philosophy.

The necessary subroutines to implement OPCON are outlined in section 2.4. The required Jacobian matrices, f_x , f_u , can be easily deduced from the model equations outlined in section 3.1.1. Formulation of the objective function is performed by addition of the new state variable given by:

$$\dot{x}_{n+1} = (T_T - T_T^*)^2 + (T_B - T_B^*)^2 ; \quad x_{n+1}(0) = 0 \quad (4.4)$$

Hence, the objective function, $F(t_f)$, becomes:

$$F(t_f) = x_{n+1}(t_f) \quad (4.5)$$

The gradient of the objective function with respect to the eleven dimensional state at the final time is then:

$$F_x(t_f) = [0,0,0,0,0,0,0,0,0,0,1] \quad (4.6)$$

The differential state and adjoint equations were integrated using a fourth order Runge-Kutta method. Although this is contrary to the numerical procedures outlined in section 2.3.2, the loss of computer time is not considered serious because of the low model dimensionality.

Three types of control problems were solved for the debutanizer: maintain set points in the face of feed changes; effect a set point change under constant feed conditions; effect a set point change accompanied by a feed change. The latter represents the feed changeover problem whereas the first two are of general control interest. Table 4.1(a) outlines the various optimal control runs with reference to the corresponding figures illustrating the results. Initial steady state conditions for these runs are shown in Table 4.1(b). For feed changeover problems,

TABLE 4.1(a) SUMMARY OF OPTIMAL CONTROL RUNS FOR DEBUTANIZER

Problem Type	Run No.	Initial Conditions (see Table 4.1(b))	Changed Variables	Results
Regulatory	DB1	B	F	Fig. 4.2
	DB2	B	T _F	Fig. 4.3
	DB3	B	z _F	Fig. 4.4
Servo	DB4	B	T _T	Fig. 4.5
	DB5	B	T _T , T _B	Fig. 4.6
Feed Changeover	DB6	A	F, T _T , T _B	Fig. 4.7
	DB7	A	F, T _T , T _B	Fig. 4.8
	DB8	B	T _F , T _T , T _B	Fig. 4.9
	DB9	A	F, z _F , T _T , T _B	Fig. 4.10

TABLE 4.1(b) INITIAL CONDITIONS FOR OPTIMAL CONTROL RUNS

Variable	Condition A	Condition B
Feed Flowrate, F , (tonnes/hr)	65	55
Feed Temperature, T_F , ($^{\circ}\text{C}$)	190	192
Feed Light Component Concentration, z_F	.35	.35
Reflux Rate, R , (tonnes/hr)	75	25
Fuel Rate, Q , (tonnes/hr)	.35	.25

Figure 4.2 Debutanizer Regulatory Problem (Run DB1)Upsets: $F : 55 \text{ t./hr.} \rightarrow 60 \text{ t./hr.}$ at $t = .5\text{hr.}$ $I_{ss} = 0.313$

—X— Set Point Trajectory
 — Optimal Control Responses; $I = 0.043$
 ○ Initial Controls

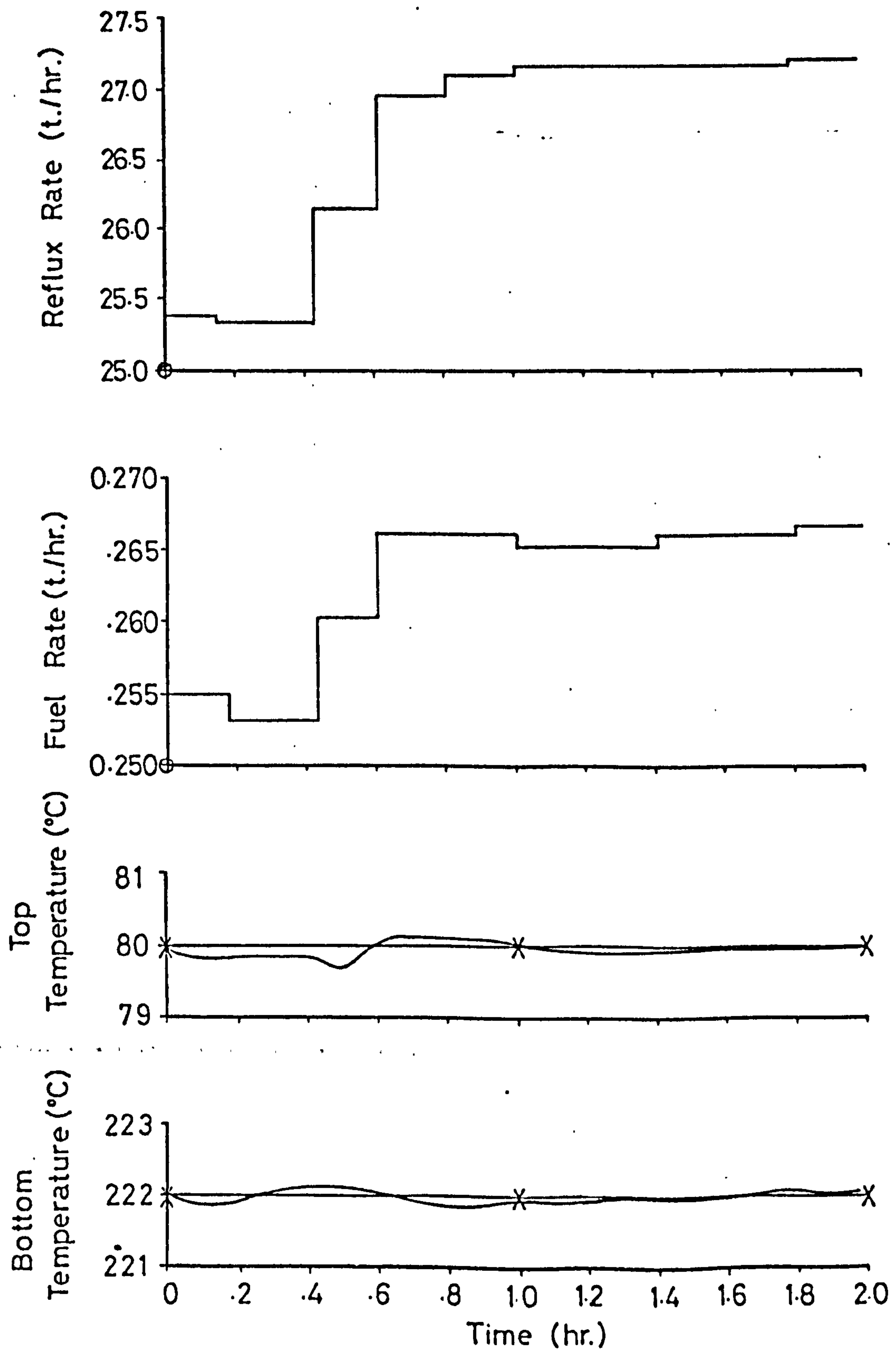


Figure 4.3 Debutanizer Regulatory Problem (Run DB2)Upsets: $T_F : 192^{\circ}\text{C} \rightarrow 185^{\circ}\text{C}$ at $t = .5$ hr. $I_{ss} = 2.34$

—x— Set Point Trajectory
 — Optimal Control Response; $I = .053$
 ⊗ Initial Controls

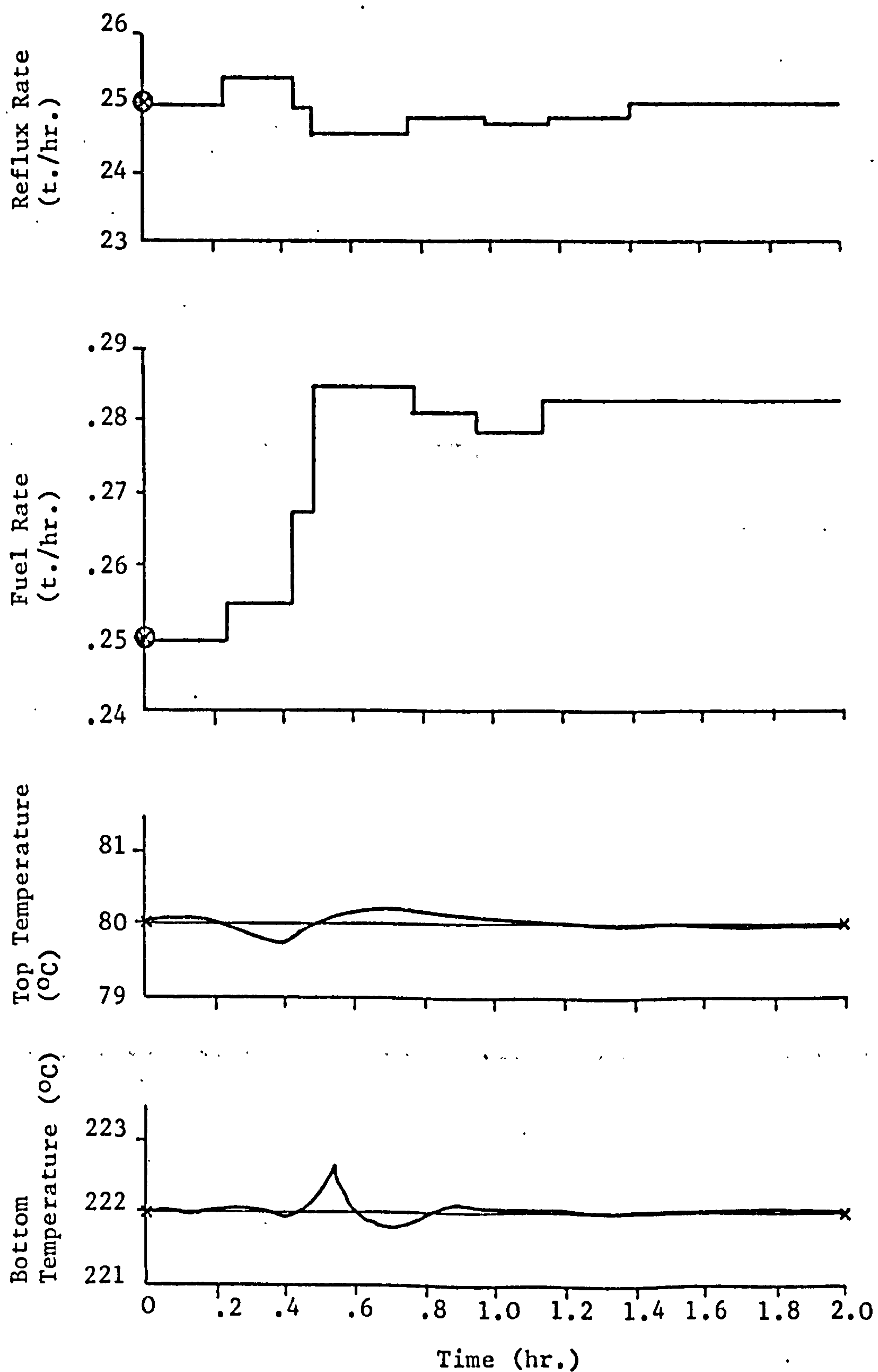


Figure 4.4 Debutanizer Regulatory Problem (Run DB3)Upsets: $z_F : .35 \rightarrow .38$ at $t = .5$ hr. $I_{ss} = 2.897$

—X—

Set Point Trajectory

—

Optimal Control Response; $I = 0.095$

○

Initial Controls

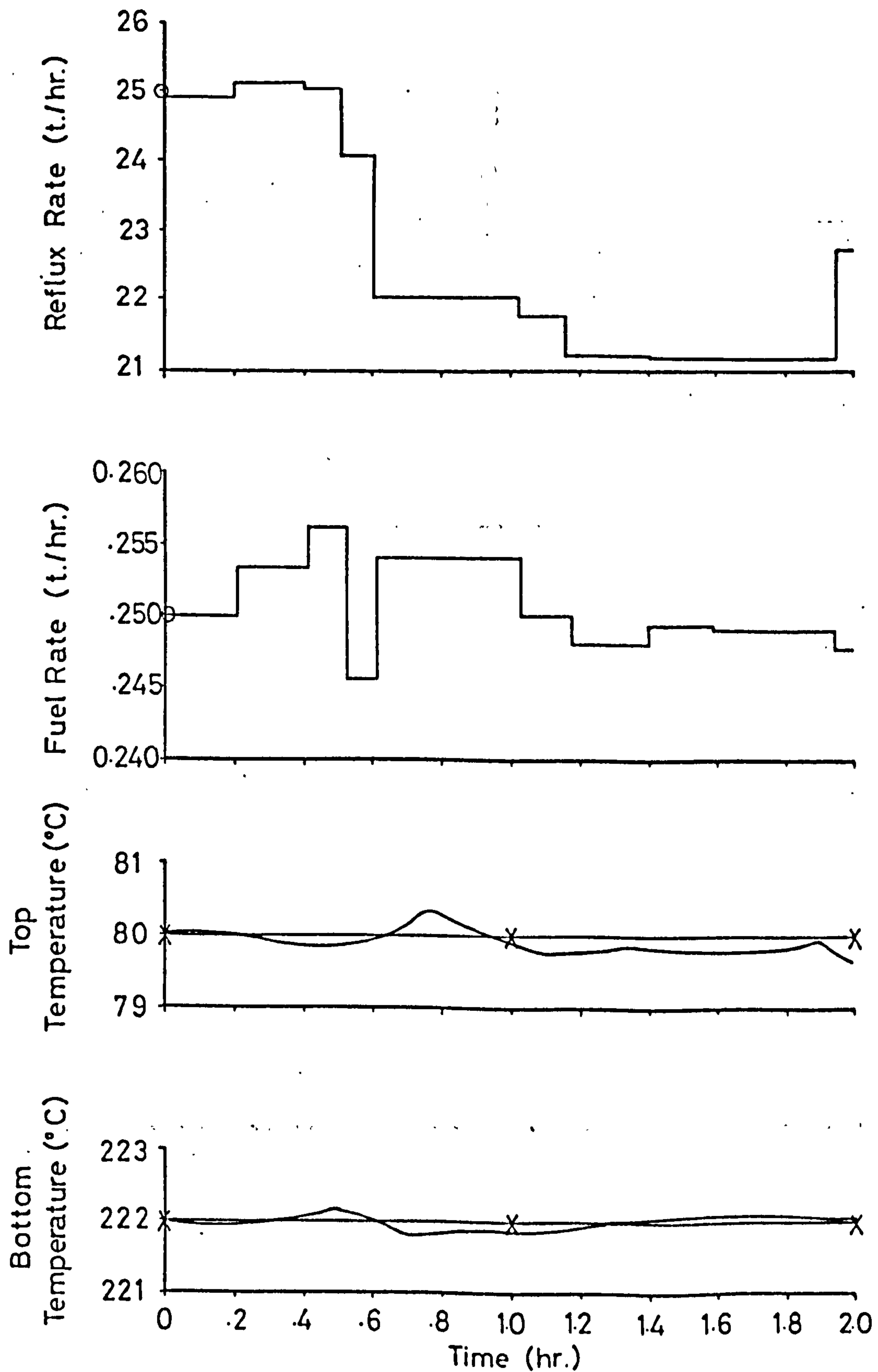


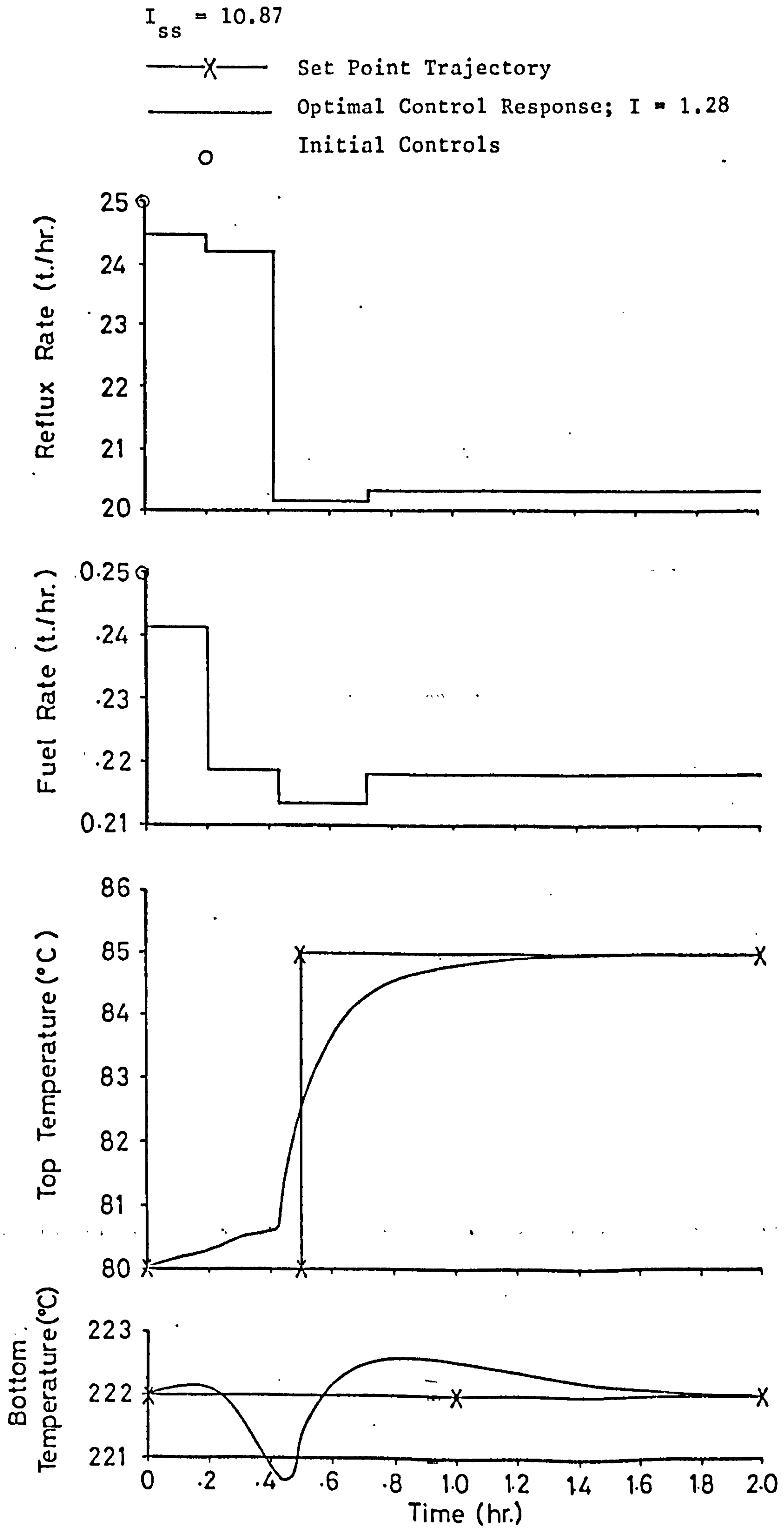
Figure 4.5 Debutanizer Servo Problem (Run DB4)

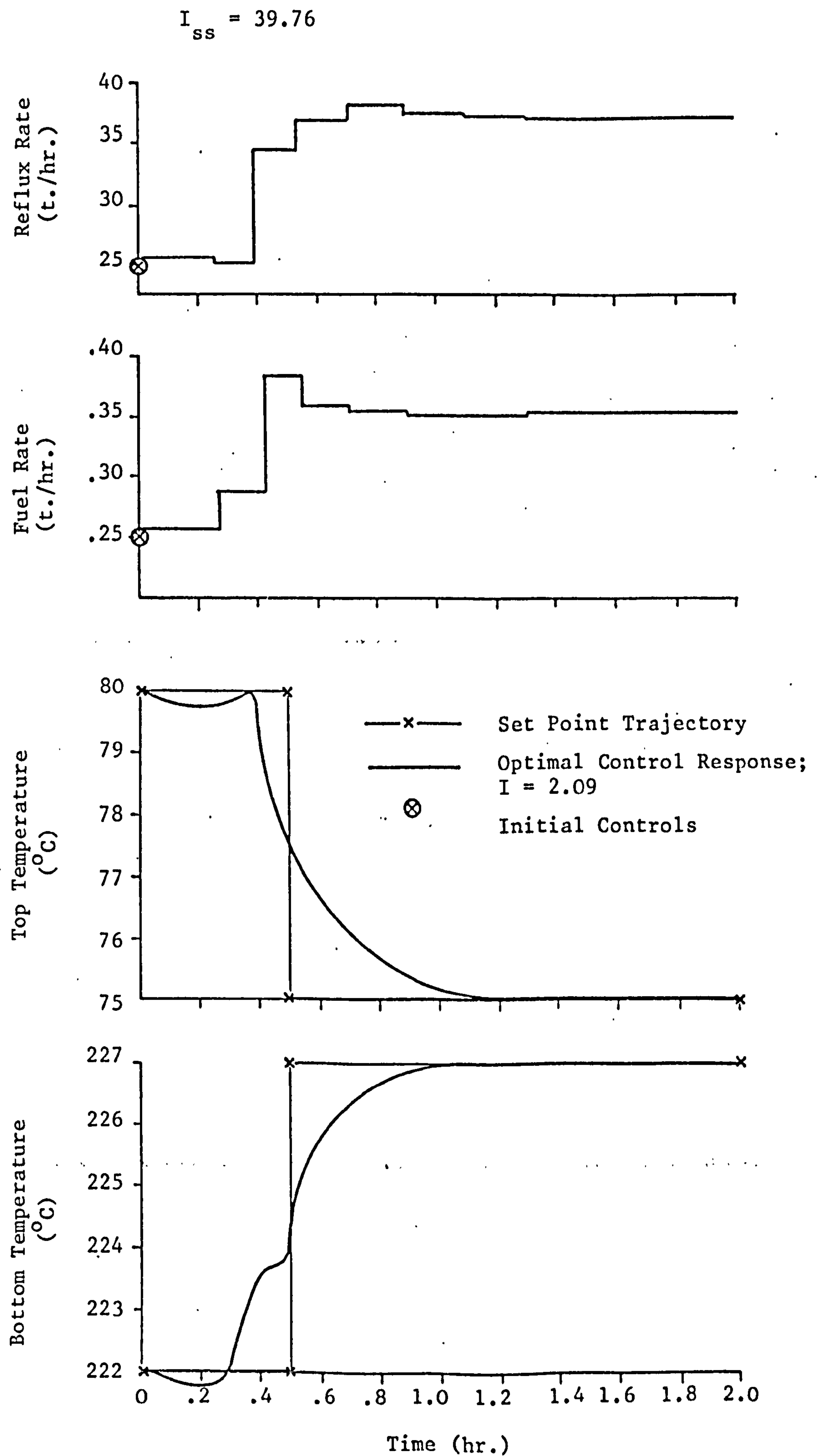
Figure 4.6 Debutanizer Servo Problem (Run DB5)

Figure 4.7 Debutanizer Feed Changeover Problem

(Run DB6)

Upsets: $F : 65 \text{ t./hr.} \rightarrow 70 \text{ t./hr.}$ at $t = 0 \text{ hr.}$

—X— Set Point Trajectory

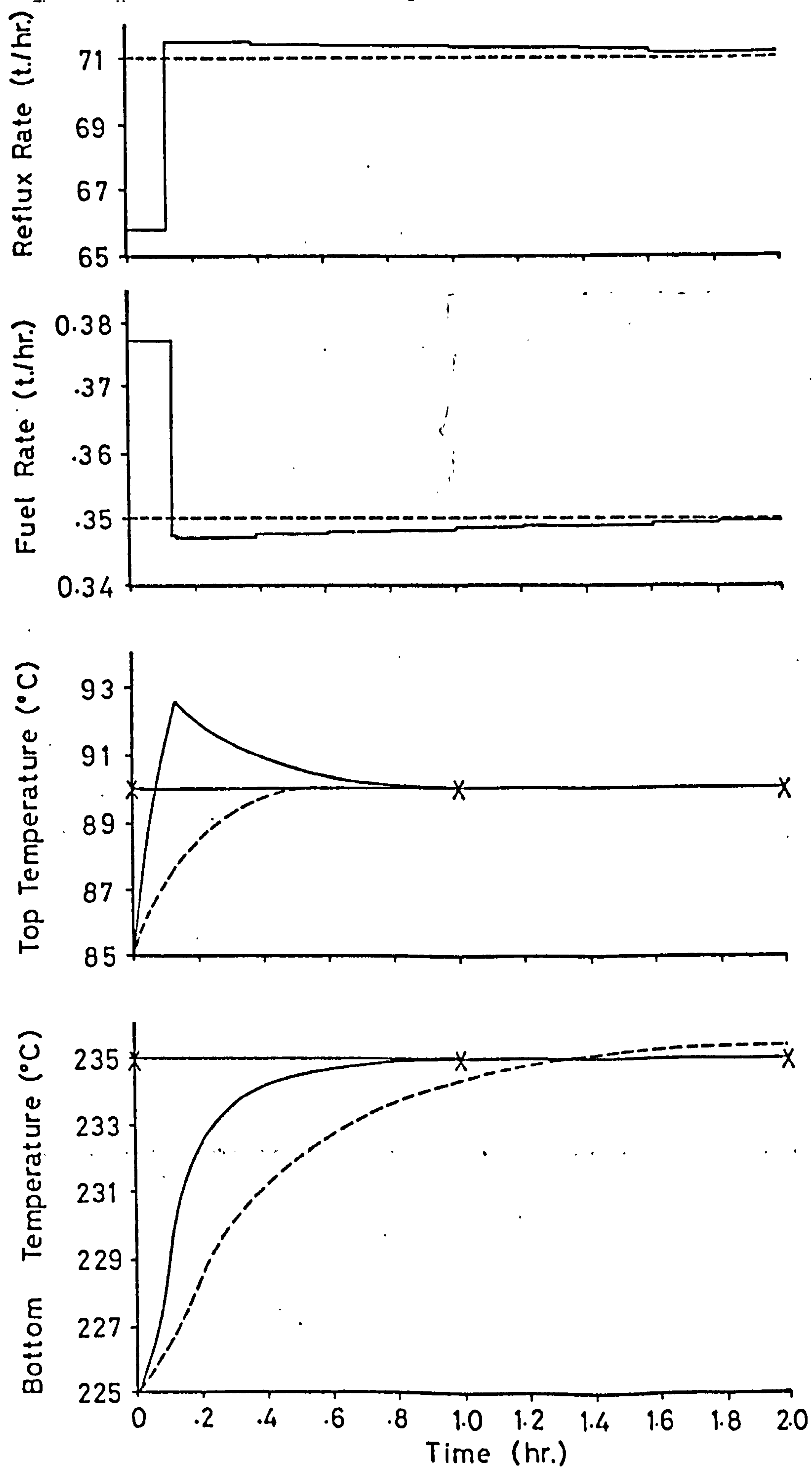
- - - Final Steady State Control Response; $I_{ss} = 23.40$ — Optimal Control Response; $I = 10.65$ 

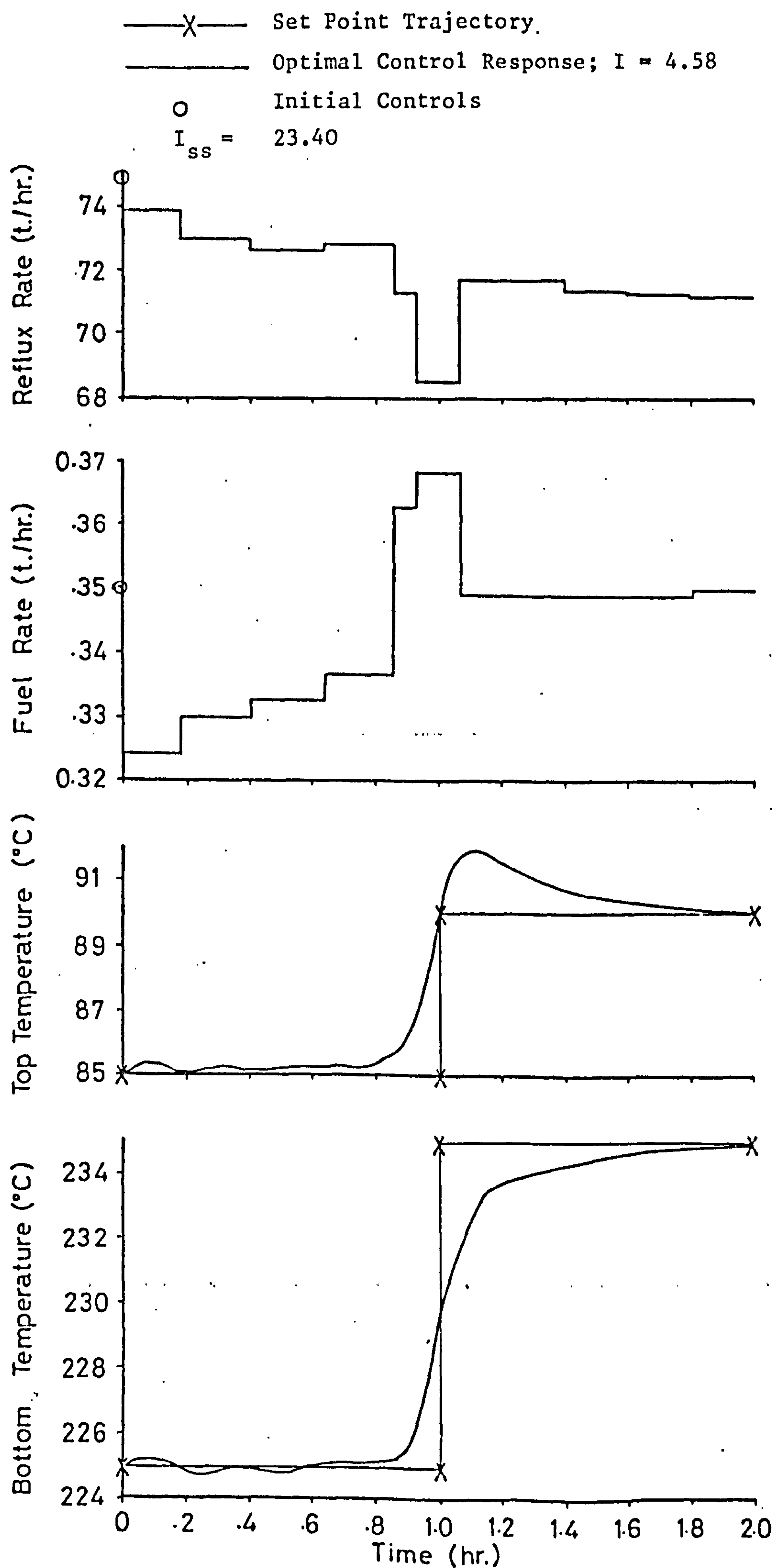
Figure 4.8 Debutanizer Feed Changeover Problem (Run DB7)Upset: $F : 65 \text{ t./hr.} \rightarrow 70 \text{ t./hr.}$ at $t = 1.0 \text{ hr.}$ 

Figure 4.9 Debutanizer Feed Changeover Problem (Run DB8)

Upsets: $T_F : 192^{\circ}\text{C} \rightarrow 205^{\circ}\text{C}$ at $t = 0.5$ hr.

$$I_{ss} = 181.49$$

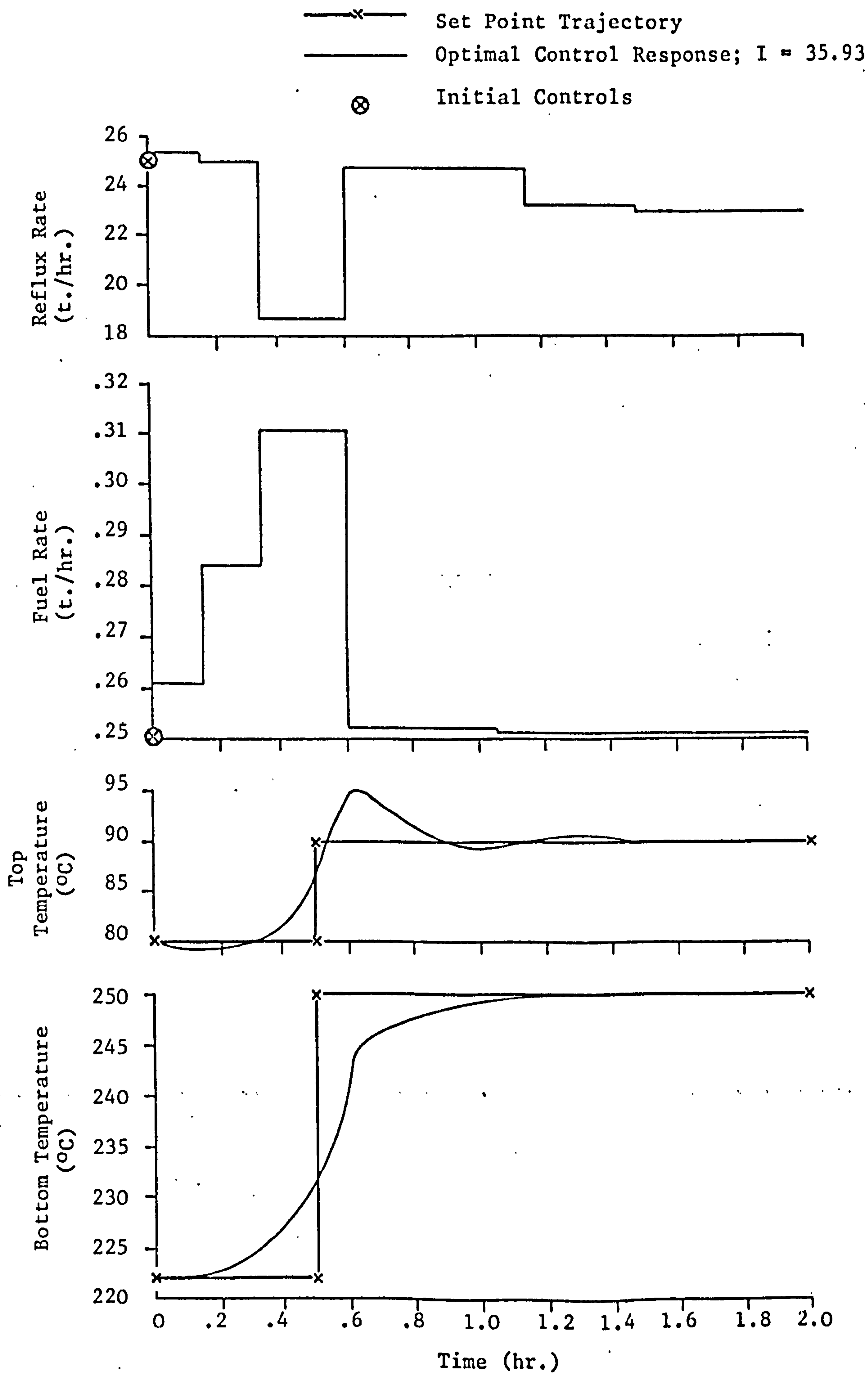
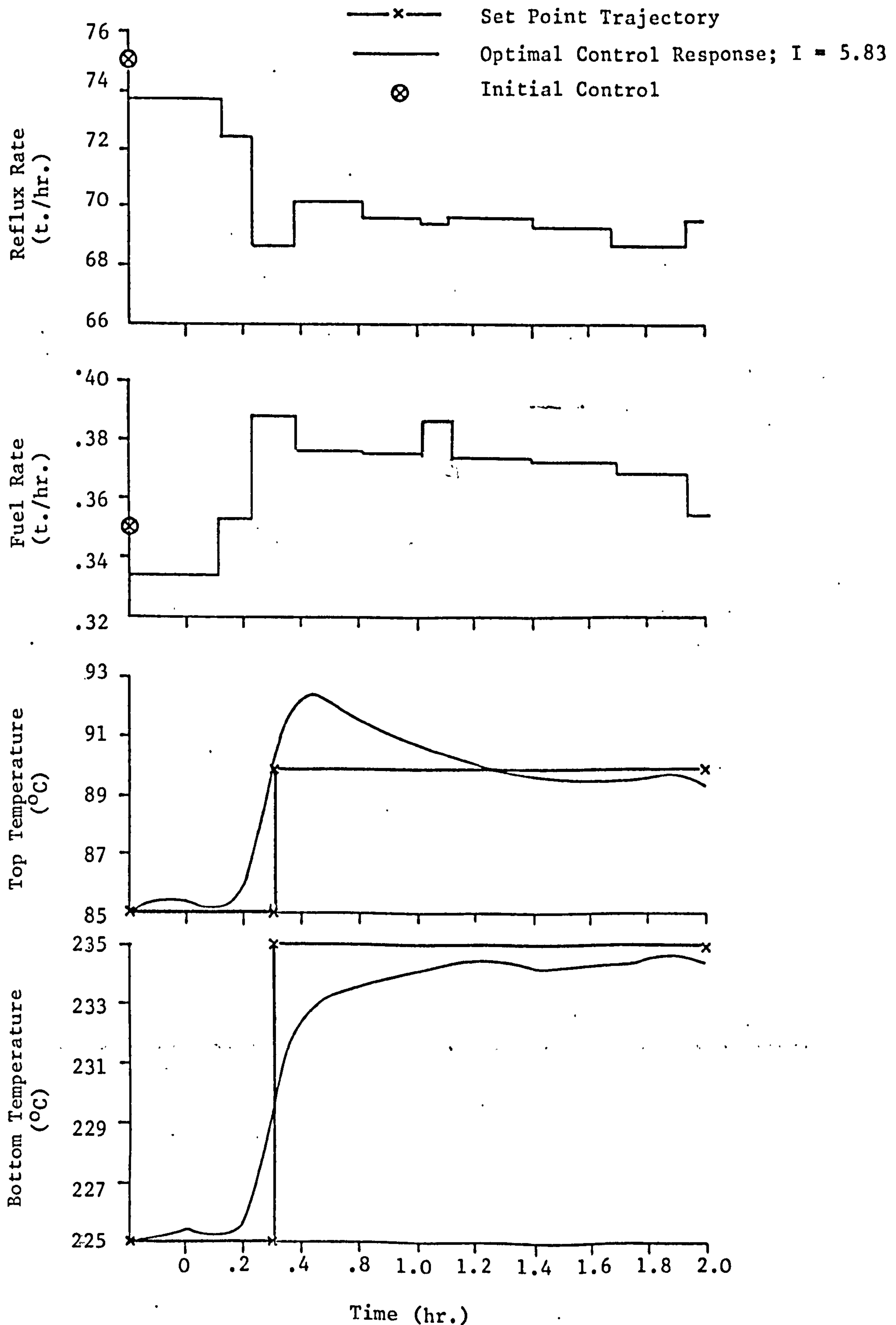


Figure 4.10 Debutanizer Feed Changeover Problem (Run DB9)Upsets: F : 65 t./hr. $\rightarrow$ 70 t./hr. at $t = .5$ hr. z_F : .35 $\rightarrow$.39 at $t = .5$ hr.

$$I_{ss} = 29.95$$



set point switches were scheduled to occur as the new feed entered the column, whereas a priori set point trajectories were assigned for servo problems. For the calculation of optimal controls, starting control trajectories were taken as steady state controls required to achieve the instantaneous set points with the resulting objective function shown as I_{ss} . Control bounds were put at physically realistic levels but these were never encountered in any of the runs. The number of control intervals (NCI) was chosen as 10, and the final time was set at 2.0 hours (approximately 6 system time constants). Only two state variables appear in the objective function, and this is equal to the number of degrees of freedom for the system. Therefore, as discussed in section 3.3.3, no final steady state control constraint was imposed.

Results for the regulatory problems are given in Figures 4.2-4.4. Excellent control of the set points is obtained by allowing the controls to move between initial and final values via a first order lag from the upset time. This is physically understandable, since feed disturbances do not immediately affect product qualities but rather are lagged through the column holdup and by mass transfer mechanisms. Consequently, control action should be similarly lagged. From Figure 4.2 and 4.3 note that the time constant for the fuel lag is shorter than that of the reflux lag. Also, by comparison of Figure 4.2 and 4.4, it is evident that reflux lags for feed composition changes are longer than those for feed rate changes which also makes physical sense; mass transfer processes are slower than hydraulic ones.

Figure 4.5 and 4.6 illustrate solutions to servo control problems. Optimal controls for a top temperature decrease and a bottom temperature increase are shown in Figure 4.6. Note that although the improvement over steady state control is large, the controls do not demonstrate any extreme action. The reason for this trend hinges upon the role of interaction between the two controllers. When set points change in opposite directions, control actions tend to oppose each other. For the problem considered in Figure 4.6, more extreme action on the reflux (i.e. a higher rate at 0.4 hours) would cause a faster decrease of the top temperature, but at the expense of sending more lights down the column to counteract the bottom temperature change. This accounts for the high value of the objective function resulting from application of steady state control. Therefore, the necessary compromise in control action to prevent such behaviour is reflected through a sluggish set point change.

These trends are also exhibited in the servo problem illustrated in Figure 4.5 in which the top temperature is to increase without any change in the bottom set point. Because of the interactions, the top temperature change cannot be implemented without affecting the bottom response. The fuel rate is first dropped causing a decrease in the bottom temperature. Then, when the reflux is dropped to facilitate the top set point change, the bottom temperature increases beyond its set point before returning to steady state. In this manner, by positioning the bottom response about its set point, the overall squared deviations are minimized.

Solutions to typical feed changeover problems are shown in

Figures 4.7-4.10. The system response for increases in the bottom and top temperatures accompanied by a feed rate upset at time zero is illustrated in Figure 4.7. Application of final steady state controls resulted in an objective function of 23.40 compared with 10.65 using the optimal controls. These controls took the form of extreme action for a short period to time followed by some compensating control in order to achieve the final steady state. Savings were made because the bottom temperature response was faster at the expense of the top temperature overshooting its new set point. The run shown in Figure 4.8 was performed under the same conditions except that the occurrence of the upset was known one hour in advance. Although the same shape of the transient curves prevail, the lower objective function value (4.58 vs. 10.65) reflects the better positioning of the responses about the set point trajectory.

Figures 4.9 and 4.10 illustrate feed temperature and feed composition coupled with feed rate changover problems respectively. Even though large set point changes are associated with the temperature changeover, the response curves maintain the general form common to the previous examples. From Figure 4.10, it can be seen that OPCON has not reached convergence as demonstrated by the deviation from steady state control at the final time. However, this is not considered serious since convergence to the final steady state control would provide negligible contribution to the objective function.

For all the feed changeover problems considered so far, set point specifications were changed at the upset time and it should be noted that this is not necessarily the optimal switching

location. The optimal switch position can be found naturally using optimal product stream fractioning policies outlined in section 3.2.2. Using these procedures, it can easily be shown that the set point at any time should be chosen as the one closest to the product stream temperature. Runs DB7-DB9 were repeated (Runs DB7(a)-DB9(a)) using the optimal set point switching rule and the response curves are given in Figures 4.11-4.13. Starting control trajectories consisted of initial steady state controls followed by a switch to final steady state controls at the upset time with the resulting objective function shown as I_{ss} . Although the position of the temperature trajectories has changed, the general shape of the curves has remained unaltered. For example in Run DB9(a) the reflux rate is lowered prior to the upset, causing both temperatures to increase. The top temperature overshoot is limited by the effect of the lighter feed that is entering the column, rather than by control action as was the case in Run DB9. For all three runs, the optimal objective function values have not changed to any great extent. However, application of steady state control in connection with optimal set point switching policies resulted in a much lower objective function value than that obtained from use of identical control with a priori switching trajectories. In fact, optimal control only reduces the steady state control objective function value by a factor of approximately two. This indicates that the combination of final steady state control with optimal set point switching policies yields a satisfactory control. There is physical justification for this observation. During feed

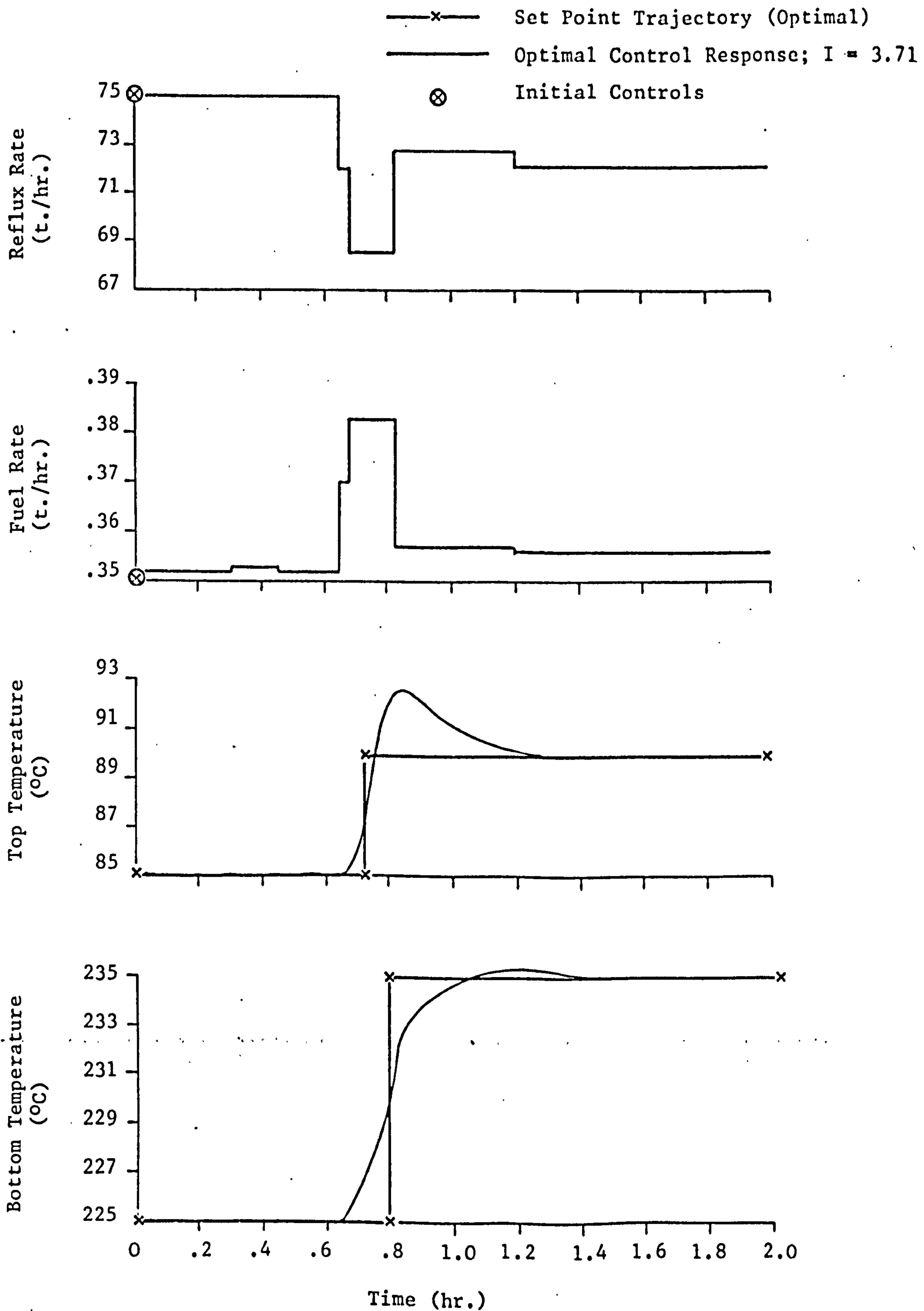
Figure 4.11 Debutanizer Feed Changeover Problem (Run DB7(a))Upsets: $F : 65 \text{ t./hr.} \rightarrow 70 \text{ t./hr.}$ at $t = .5 \text{ hr.}$ $I_{ss} = 8.90$ 

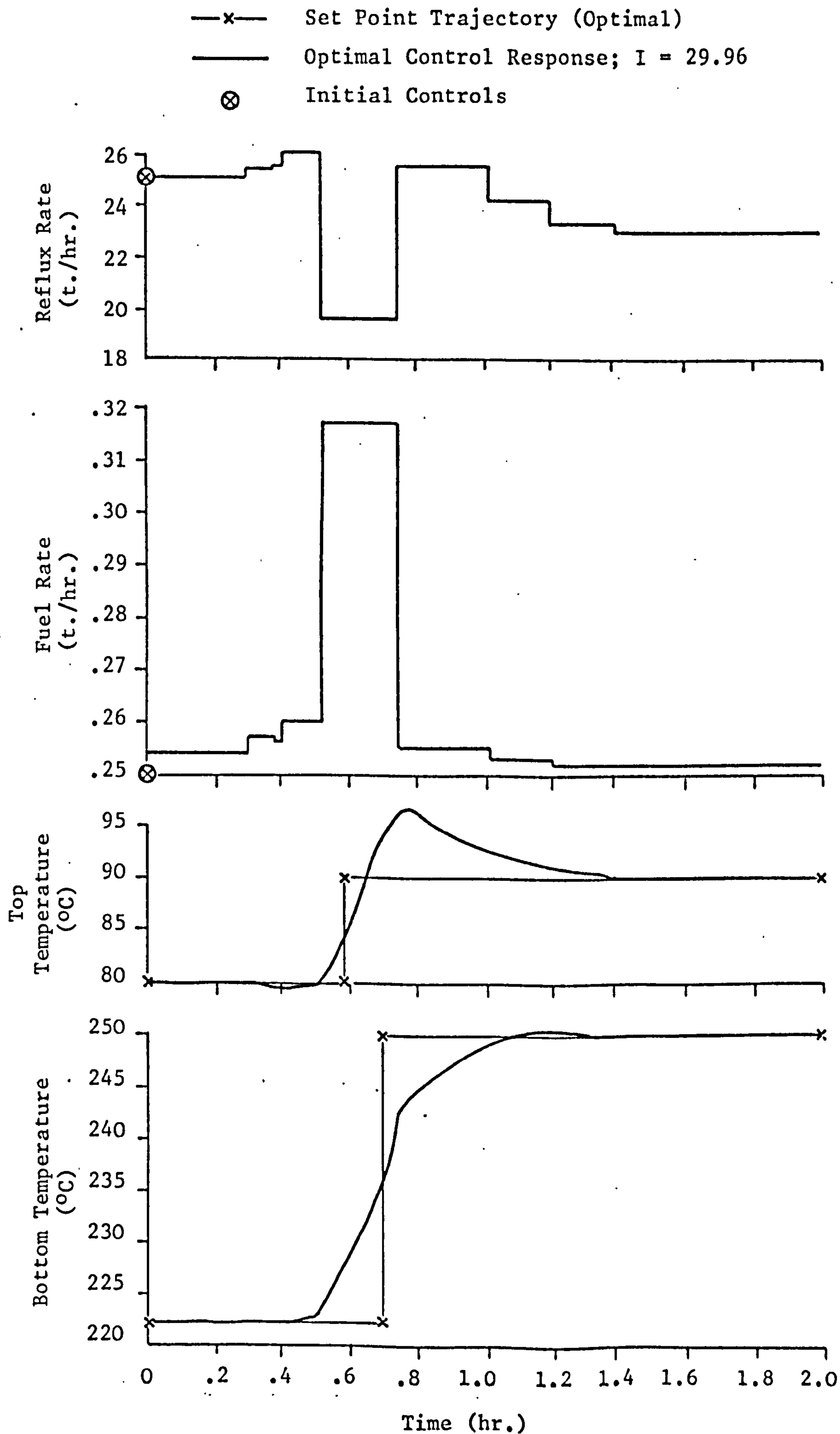
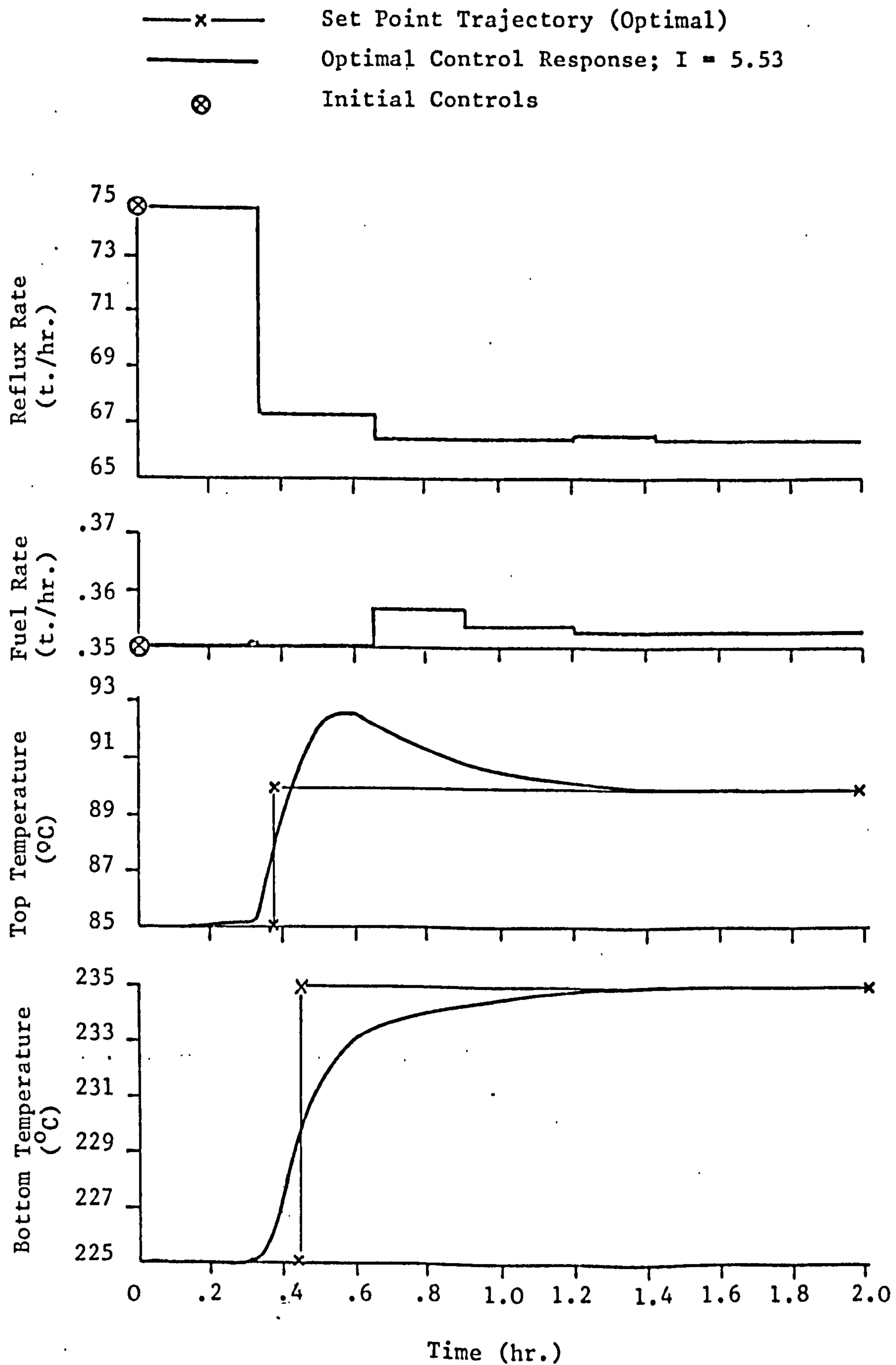
Figure 4.12 Debutanizer Feed Changeover Problem (Run DB8(a))Upsets: T_F : $192^{\circ}\text{C} \rightarrow 205^{\circ}\text{C}$ at $t = .5$ hr. $I_{ss} = 64.01$ 

Figure 4.13 Debutanizer Feed Changeover Problem (Run DB9(a))Upsets: F : 65 t./hr. $\rightarrow$ 70 t./hr. at $t = .5$ hr. z_F : .35 $\rightarrow$.39 at $t = .5$ hr. $I_{ss} = 7.42$ 

changeovers, top and bottom set points change in the same direction because the new feed coming from the top of the main column is either lighter or heavier in terms of both pseudo-components. Hence, reflux and heating actions complement each other. For example, decreases in the reflux flow or increases in the fuel rate serve to increase both top and bottom temperatures. However, as already discussed, set point changes in opposite directions rely on control actions that oppose each other.

4.2.3 Implementation Aspects

Now that the optimal responses have been obtained, an on-line control structure is sought that would lead to an approximation of the off-line responses. Of the three types of problems considered in section 4.2.1, the feed changeover one is of prime importance. The very fast set point changes were effected by extreme control action which was possible because of the interactions; the direction of the set point changes were such that controls supported each other. Implementation of policies based upon these trends would involve the choice of extreme control levels together with the timing of their application. These could be determined a priori from the open-loop studies and used as a feedforward control for the changeover period. However, this would require a dynamic optimization for every changeover, and even if this were possible, the effect of model inaccuracies often degrades the performance of purely feedforward control strategies, as demonstrated by Nieman and Fisher (1973) for a pilot plant evaporator.

It is clear that some feedback is necessary in any proposed algorithm. Observation of responses in Figure 4.7- Figure 4.13 reveals a potentially useful feedback switching rule. In every case, extreme control conditions are relaxed when the overshoot of the top temperature trajectory is approximately equal to the undershoot of the bottom response. With hindsight, one can develop some theoretical justification for such a law. It can be easily shown that if the rates of increase of the top and bottom temperature are the same, then the instantaneous value of the objective function, given by the right hand side of Eq.(4.4), passes through a minimum at the undershoot equals overshoot condition. If the objective function contains non-equal weighting for the top and bottom temperatures, then the minimum condition occurs when the correspondingly weighted overshoots and undershoots are equal. At this point, if application of extreme control is continued, instantaneous values of the objective function begin to increase, and the return to the new steady state becomes progressively more difficult. Similarly, higher objective function values would result if extreme control action was relaxed before encountering the overshoot equals undershoot condition.

This switching law can be used as a basis for an on-line control algorithm which consists of feedforward control levels together with feedback switching times, as follows:

- (i) Apply existing feedback control until the upset time.
- (ii) Apply extreme control until the overshoot of one temperature response is equal to the undershoot of the other.
- (iii) Apply final steady state control to reach the new set points.

Some explanations concerning the algorithm are in order. Implementation of final steady state control, rather than standard three-term feedback control, to attain the new steady state seems unnecessary. However, at the point of extreme control relaxation, application of feedback control would lead to strong interactions between the top and bottom of the column. For example, from Figure 4.11, at the overshoot equals undershoot condition, a feedback controller on the bottom would demand more fuel (which is contrary to the optimal results) and thus counteract the actions of the reflux control that causes the top temperature to decline.

The overshoot equals undershoot rule corrects for any approximation in values of the extreme control levels. If the control is too extreme, this condition would be satisfied earlier than in the optimal case. Final steady state control would be switched on sooner at the expense of bringing the temperatures a further distance to their new set points.

Conversely, a less extreme control will result in implementation of final steady state control later than in the optimal case. This feedback nature of the algorithm will also compensate for model inaccuracies.

The problem still remains of choosing the extreme control levels a priori. Application of final steady state control for the entire period from the upset time has been shown to yield satisfactory objective function values. For this control policy, the undershoot equals overshoot condition will never be satisfied since the temperatures approach the new set points asymptotically. If the extreme control levels which emerged from the optimal control studies were implemented within the context of the proposed

algorithm, the optimal objective function value would not be achieved. This is due to the fact that some compensating control, rather than final steady state control, is applied at the undershoot equals overshoot condition (see Figure 4.11, Figure 4.12). Rather than add this extra complication to the proposed algorithm, it may be worthwhile to examine policies that use less extreme control action and hence require no compensating action. Run DB7(a) was performed using the proposed algorithm and various levels of extreme control. For the purposes of comparison, an optimality approach factor, OAF, is defined as:

$$\text{OAF} = \frac{I_{ss} - I_{so}}{I_{ss} - I_o} \quad (4.7)$$

where subscripts so and s refer to sub-optimal and optimal conditions respectively. Thus, steady state and optimal controls have OAF values of 0 and 1 respectively. Results are presented in Table 4.2. Extreme control levels have been varied from final steady state control to those appearing in the optimal results.

From Table 4.2 it is clear that not very much "extreme" action is required to achieve high OAF values. The sensitivity of the objective function to the choice of control level is small, until the control becomes too extreme. This indicates that a correlation which relates the value of the extreme control levels to the final steady state controls and the size of the set point changes should be robust. The following relationship was developed from observations of the optimal responses:

TABLE 4.2 OPTIMALITY APPROACH FACTORS FOR PROPOSED SUB-OPTIMAL
ALGORITHM WITH VARIOUS EXTREME CONTROL LEVELS

Test Problem: Run DB7(a)

$$I_{ss} = 8.90$$

$$I_o = 3.71$$

Extreme Control Levels		Objective Function, I	OAF
R	Q		
72.04	.356	8.90	0
71.40	.361	5.39	.675
70.80	.366	4.76	.797
70.20	.371	4.86	.776
69.6	.376	5.31	.691
69.0	.381	5.99	.559
68.5*	.383*	6.74	.416

* Taken from Optimal Response (See Fig. 4.11)

$$R_e = R_f - (.002 \Delta T_T + .001 \Delta T_B) \quad (4.8)$$

$$Q_e = Q_f + (.002 \Delta T_T + .0016 \Delta T_B) \quad (4.9)$$

where ΔT_T is the top temperature set point change, ΔT_B is the bottom temperature set point change, and subscripts e, f refer to extreme and final steady state conditions respectively. The constants in Eq.(4.8) and (4.9) were simply approximated in order to demonstrate the robustness of the optimal switching law. Runs DB7(a)-DB9(a) were repeated utilizing this control law in conjunction with the proposed on-line algorithm and the results are shown in Table 4.3. Note that all the sub-optimal policies produce significantly better objective functions than those obtained from application of final steady state controls. The apparently poor OAF value corresponding to Run DB9(a) is not considered serious because of the small difference between steady state and optimal objective function values.

For the regulatory problem, where set points are to be maintained in the face of upsets, the optimal responses indicate that controls should move from one steady state to another via a first order lag. This could easily be implemented using DBSS to predict the final steady state controls for the new feed conditions. When a disturbance is sensed, control lags would be supervised for a short period of time by a feedforward system after which existing feedback control would be switched back on. Estimates of the first order time constants can be obtained from the optimal responses, but these would inevitably be tuned on the plant. This structure is similar to that recommended by Shinskey (1967) for feedforward/feedback control of distillation columns.

The suggested control structures for the changeover and regulatory problems possess a common benefit: they both interface

TABLE 4.3 PERFORMANCE OF SUB-OPTIMAL CONTROL LAW

Run	R_f	Q_f	R_e	Q_e	I_{ss}	I_o	I_{so}	OAF
DB7(a)	72.02	.355	70.57	.364	8.90	3.71	4.55	.838
DB8(a)	22.97	.252	21.87	.263	64.01	29.96	41.13	.672
DB9(a)	66.40	.353	65.07	.362	7.42	5.53	6.53	.471

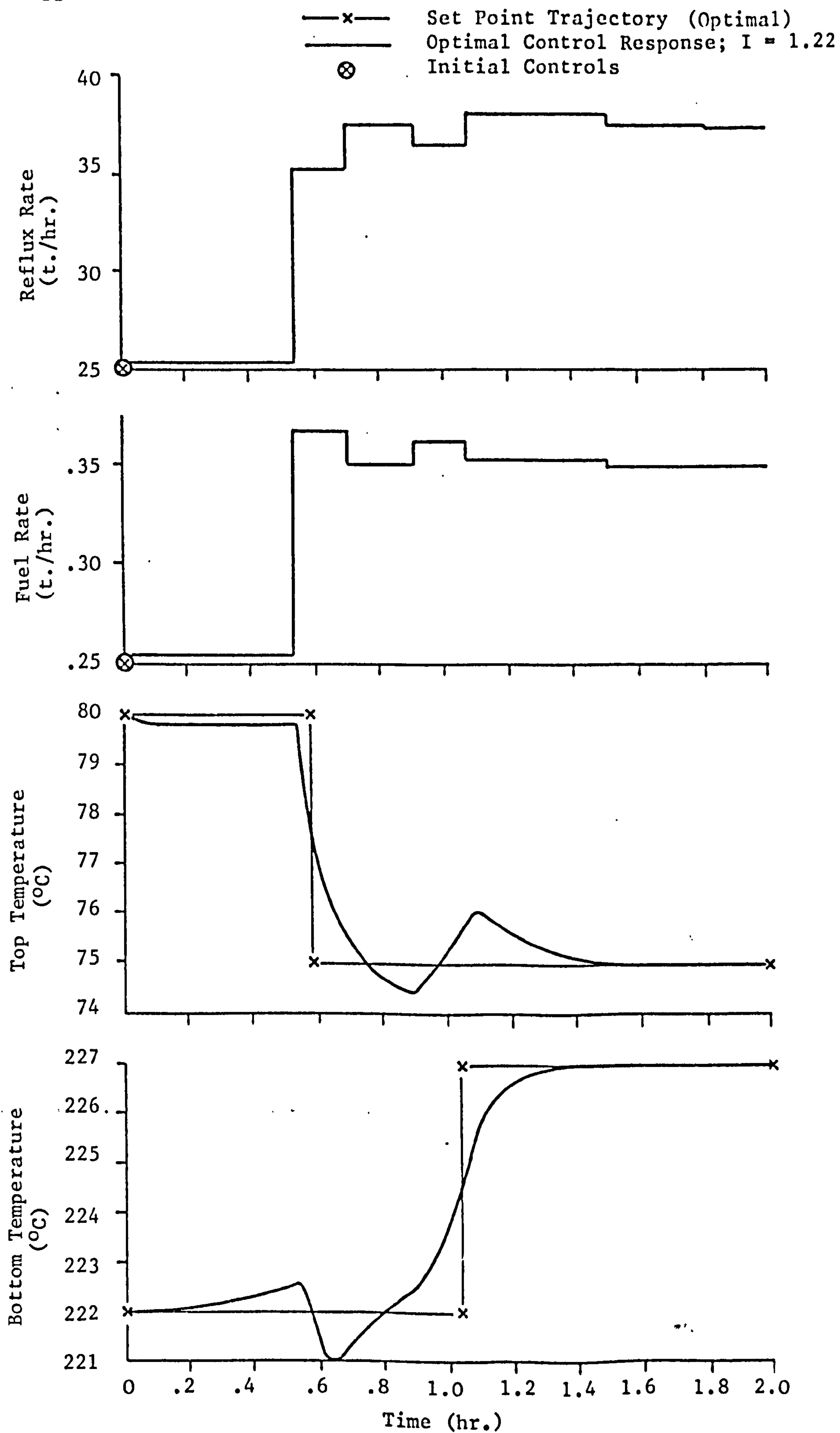
and operate in conjunction with existing feedback hardware. The feedforward strategy requires a small computer to calculate steady state control levels using DBSS. Alternatively, control values could be determined a priori over the spectrum of feed and operating conditions in order to provide control tables for the operators.

The servo problem, in which set points are to change under constant feed conditions, is a more complicated case. When the set point changes are in the same direction, strategy identical to that suggested for the feed changeover problem can be utilized. However, when the set points are to move in opposite directions, control actions no longer complement each other, as demonstrated in Run DB5. The results from Run DB4 indicate a control philosophy that could be useful in these situations. The controls were manipulated so that both ends of the column became heavier together when the top set point changed. This could not occur in Run DB5 since the set points were constrained to switch at the same instant in time. More latitude could be obtained if the set point switches were allowed to float during the optimization calculations according to the optimal switching policy.

These speculations are confirmed by the results of Run DB5(a) which was performed under the conditions of Run DB5 except with application of the optimal set point switching law. The results are illustrated in Figure 4.14. The starting trajectory for this run was taken as a switch to final steady state control at 0.5 hours. The corresponding objective function has been reduced by a factor of six by the optimal controls which indicates that the application of final steady state control does not yield satisfactory response. For the majority of the run, column contents.

Figure 4.14 Debutanizer Servo Problem (Run DB5(a))

$$I_{ss} = 7.67$$



do move lighter and heavier together. The controls initially cause the bottom temperature to increase, but it drops sharply when the sudden jump in the reflux and fuel rate takes place to force a fast top temperature change. The minimum in the bottom response hinges on the fact that heat transfer lag associated with a fuel increase is longer than the time taken for increased reflux rate to reach the bottom of the column. Since the bottom temperature change cannot be implemented without affecting the top response, the top temperature overshoots its new set point. In this manner, the trajectory is centred about the new set point when the bottom temperature change is effected. It is interesting to note that the first portion of response in Run DB5(a) during the top set point change resembles Run DB4 in which the top temperature changes while the bottom set point remains fixed. Benefit from the control philosophy of moving both ends of the column in the same direction is reflected in an objective function value of 1.22 versus 2.09 for the constrained set point switch.

4.3. The Splitter

The bottom product of the debutanizer is processed by the splitter which produces three products: raw gasoline, benzene, and naphtha. The dynamic analysis will be based upon step changes in the feed parameters for the same reasons outlined for the debutanizer in section 4.2. Since a feed change first passes through the main column and then the debutanizer, the effect is attenuated upon entry to the splitter. Therefore, rather than examine changeover problems, emphasis will be placed on the solution to two sub-problems of interest: maintenance of set points

in the face of feed upsets and set point changes in conjunction with undisturbed feed conditions. These will prove to be valuable stepping stones for the main column studies. In order to assess the value of the optimal control results, some comparisons will be made with responses obtained from application of conventional proportional-integral controllers.

4.3.1 Steady State Analysis

Steady state analysis of the splitter involves the solution to two different problems. For given feed conditions and controls, product temperatures must be calculated. Also, for given feed conditions and product stream temperatures, the steady state controls, R , S_2 , and Q_6 are sought. The former allows the determination of initial section compositions for the dynamic optimization whereas a first approximation of the optimal controls for a given operation change is provided by the latter. These two problems will be considered in turn.

The column flow profile is uniquely defined by selection of distillate rate, D , reflux rate, R , and sidestream rate, S_2 . Starting at the top of the column, Eq.(3.16) and (3.17) can be solved in the steady state to yield:

$$L_{out} = (1 - \frac{1}{k})(L_{in} - V_{out}) + L_{in} + \frac{Q_{out}}{\lambda} \quad (4.10)$$

followed by a total material balance around each section to give:

$$V_{in} = V_{out} + L_{out} - L_{in} \quad (4.11)$$

A section-to-section calculation down the column, accounting for the sidestream drawoff and feed flows, will specify the internal flow profile. At the base of the column, the bottom product

product flow, B , is given by:

$$B = L_5 - V_6 \quad (4.12)$$

and the reboiler heat load, $-Q_6$, can be determined from Eq.(4.13) and (4.12) as:

$$-Q_6 = -\lambda \left(\frac{B}{k} - L_5 \right) \quad (4.13)$$

This leaves 12 non-linear equations in 12 unknowns (2 component concentrations per section) of the form:

$$L_{in} x_{in,j} + V_{in} y_{in,j} - L_{out} x_{out,j} - V_{out} y_{out,j} = 0 \quad (4.14)$$

with the vapour concentration in any section related to the liquid concentration by:

$$y_{ij} = \frac{\alpha_{ij} x_{ij}}{\sum_{p=1}^3 \alpha_{ip} x_{ip}} \quad (4.15)$$

where:

x_{ij} is the liquid concentration of the j th component in the i th section,

y_{ij} is the vapour concentration of the j th component in the i th section,

α_{ip} is the relative volatility of the p th component in the i th section.

The concentration of heavy component in the denominator of Eq.(4.15) can be eliminated by using:

$$x_{i3} = 1 - x_{i1} - x_{i2} \quad (4.16)$$

After allowing for blending on the feed plate, the solution to the

to the 12 non-linear equations can be found using a non-linear equation solver. For this application, the secant method of Gragg and Stewart (1976) was employed since it does not require gradients of the non-linear equations with respect to the variables. Product stream temperature changes from reference conditions can then be evaluated from the relations:

$$\Delta T_D = K_{D_1} \Delta x_{11} \quad (4.17)$$

$$\Delta T_S = K_{S_1} \Delta x_{21} + K_{S_3} \Delta x_{23} \quad (4.18)$$

$$\Delta T_B = K_{B_3} \Delta x_{63} \quad (4.19)$$

where:

ΔT is the temperature change from reference conditions,

Δx_{ij} is the change of x_{ij} from reference conditions,

K terms are known proportionality factors from identification experiments,

subscripts, D,S,B, refer to distillate, sidestream and bottoms respectively

The algorithm converges to the solution from a suitable initial estimate (e.g. linear concentration profile).

The more difficult problem is to determine the controls R , S_2 , and Q_6 for given feed conditions, reference variables, and desired temperature changes. Although the flow profile is uniquely specified by choice of R , S_2 , and Q_6 , it cannot be determined from them without iteration since the chosen controls appear at the opposite ends of the column. This can be avoided if the reboiler heat load, $-Q_6$, is replaced by the distillate

rate, D , as the independent variable. In this manner, the internal liquid and vapour rates can be evaluated directly, as outlined previously, and the desired value of Q_6 is obtained through Eq.(4.13). Now, the independent variables D, R , and S_2 , must be chosen to satisfy Eq.(4.17)-(4.19) as well as the 12 component balance equations. One method would be to add the three new equations to the previous set, the three independent variables to the set of unknown liquid concentrations, and solve the larger problem. However, a better approach is to use Eq.(4.17)-(4.19) to eliminate some of the unknowns, as demonstrated below.

Eq.(4.17) can be used to derive the following expression for x_{11} :

$$x_{11} = x_{11}^R + \frac{\Delta T_D}{K_{D1}} \quad (4.20)$$

where superscript R denotes reference conditions. Similarly, two additional liquid concentrations can be eliminated by using Eq.(4.18) and (4.19) with Eq.(4.16) to give:

$$x_{22} = 1 - x_{21} - \left[x_{23}^R + \frac{\Delta T_S - K_{S1}(x_{21} - x_{21}^R)}{K_{S3}} \right] \quad (4.21)$$

$$x_{62} = 1 - x_{21} - \left[x_{63}^R + \frac{\Delta T_B}{K_{B3}} \right] \quad (4.22)$$

The non-linear equation solver requires a routine to calculate residuals for any set of specified variables. Thus, given R, S_2, D , and the concentrations other than x_{11}, x_{22} and x_{62} , the flow

profile is first calculated, and then the residulas of the 12 component balance equations (4.14) are determined using the same subroutine as before in conjunction with the non-linear equation solver.

Sets of typical results using the digital computer program (SPSS) written to calculate the steady state are shown in Figures 4.15 and 4.16. The former illustrates changes in control parameters with x_{11} in order to maintain the sidestream and bottoms set points. As the concentration of light component in the distillate becomes larger, reflux and distillate rates are decreased while the sidestream flow is increased at a rate almost double that of the reflux decrease. This is a dangerous situation in that, at x_{11} concentrations greater than .4675, negative liquid flowrates appear below the second section (i.e. all the reflux is taken off as sidestream product). Such sensitivity is not exhibited for increases in x_{63} while maintaining top and sidestream set points, as shown in Figure 4.16. Both the sidestream and distillate remain almost flat as greater values of x_{63} are demanded. This analysis has revealed limits on the range over which the model is valid. Dynamic studies will be confined to lie within this range.

4.3.2 Dynamic Optimal Control and Implementation Apsects

Dynamic optimization was performed using an objective function of the type:

$$I = \int_0^{t_f} \{ (T_D - T_D^*)^2 + (T_S - T_S^*)^2 + (T_B - T_B^*)^2 \} dt \quad (4.23)$$

As in the case of the debutanizer equal weightings have been assumed for stream temperature deviations. For these studies, set point

Figure 4.15 Splitter Steady State Analysis

Control Parameters vs. x_{11} For Maintenance of Bottom and Sidestream Temperatures:

Feed Conditions: $F = 65 \text{ t./hr.}$

$T_F = 117.5^\circ\text{C}$

$z_{F1} = .30$

$z_{F2} = .45$

Reference Conditions:

$R_{x11} = .4661$

$R_{x21} = .3147$

$R_{x23} = .1579$

$R_{x63} = .4455$

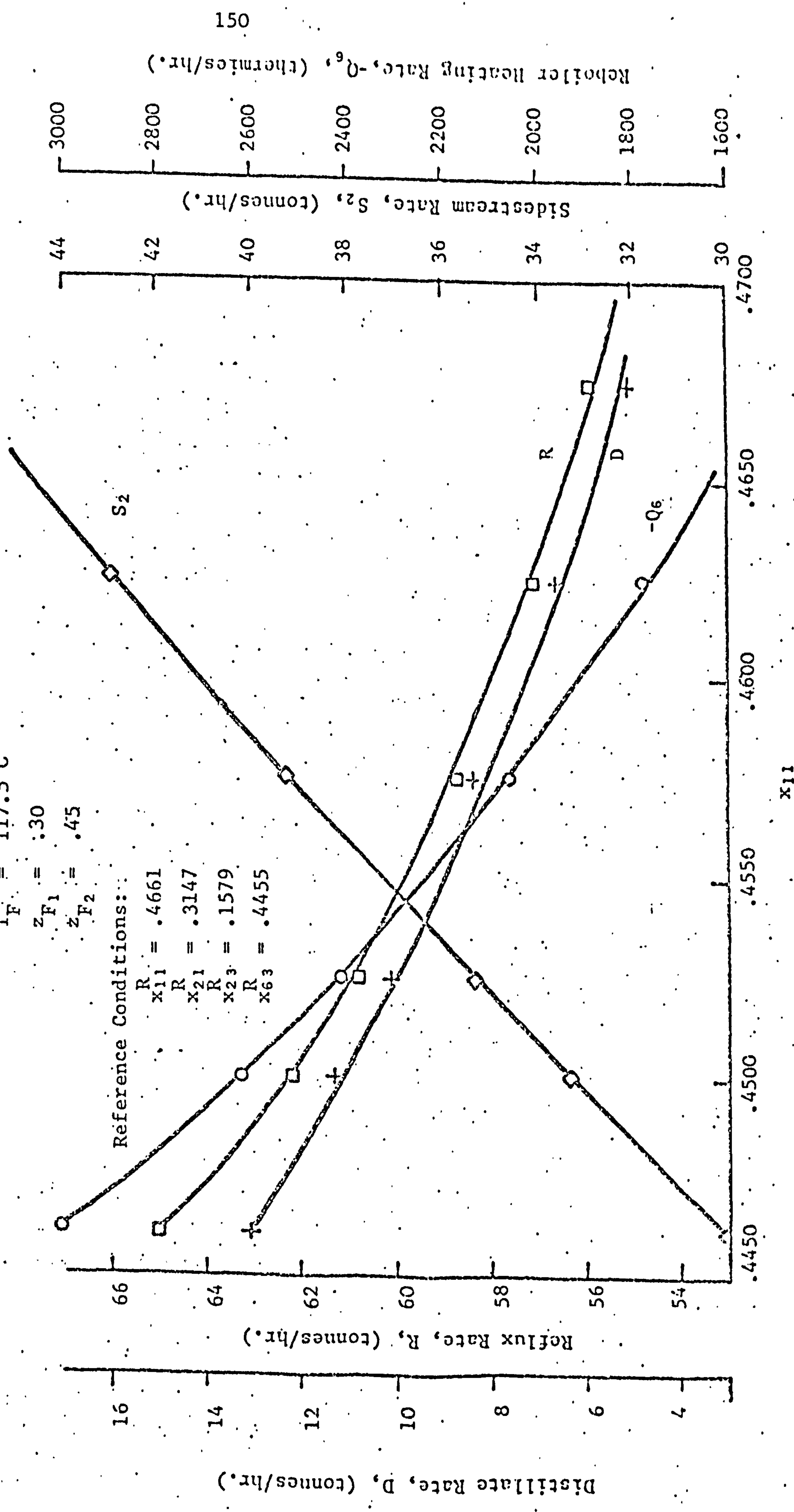
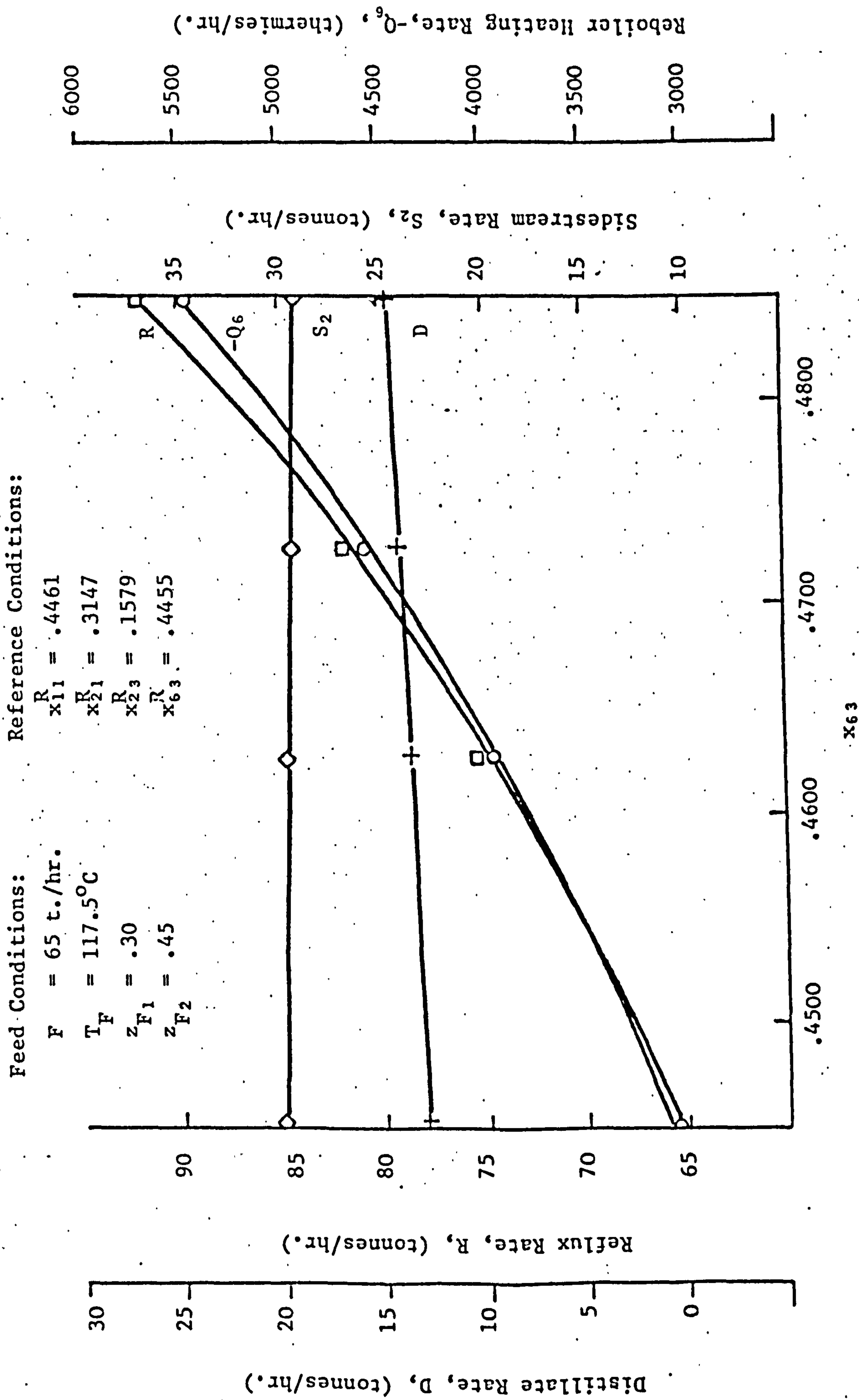


Figure 4.16 Splitter Steady State Analysis

Control Parameters vs. x_{63} for Maintenance of Top and Sidestream Temperatures:

trajectories will be assigned a priori and a value of t_f of 2 hours has been chosen.

Implementation of OPCON requires subroutines to evaluate f , f_x , and f_u . The following procedure was adopted for the preparation of these subroutines:

- (i) A typical transient response resulting from application of a simulation package was provided by British Petroleum Company Ltd. The subroutine to evaluate f was written and verified by comparison of a dynamic response with the supplied BP simulation. This response was obtained using a Runge-Kutta integration.
- (ii) Subroutines to evaluate f_x and f_u were written and verified by comparison with finite difference analysis performed on f .

Table 4.4 outlines the various optimal control runs and initial conditions for the regulatory and servo problems. For the optimal control calculations, the initial control trajectory was taken as the steady state control required to maintain the instantaneous set points. Control bounds were set at physically realistic values but these were never encountered in any runs, except for the case to be discussed later where the sidestream flowrate was purposely limited. As in the debutanizer study, the number of control intervals (NCI) was set to 10 and final steady state control was not imposed, as discussed in section 3.3.3.

Results for the regulatory problems are shown in Figure 4.17-4.19. In all figures the fuel rate fraction shown is defined as $-Q_R/6000$. It is apparent that switching to final steady state control a short time before the upset is scheduled to occur can be advantageous for feed temperature and flowrate upsets. Since flow and

TABLE 4.4 SUMMARY OF OPTIMAL CONTROL RUNS AND INITIAL
CONDITIONS FOR SPLITTER

Problem Type	Changed Variables	Results in Fig.	Run No.
Regulatory	F	4.17	SP1
	T_F	4.18	SP2
	z_F	4.19	SP3
Servo	T_D, T_S	4.20	SP4
	T_B	4.21	SP5

Initial Conditions for All Runs

F = 65.0 tonnes/hr.

T_F = 127.5 °C

z_{F1} = 0.30

z_{F2} = 0.45

D = 13.0 tonnes/hr.

R = 65.0 tonnes/hr.

S_2 = 30.0 tonnes/hr.

Q_R = -3149 thermies/hr.

Figure 4.17 Splitter Regulatory Problem (Run SP1)Upsets: $F : 65 \text{ t./hr.} \rightarrow 70 \text{ t./hr.}$ at $t = .5 \text{ hr.}$

$$I_{ss} = .340$$

$$I = .052$$

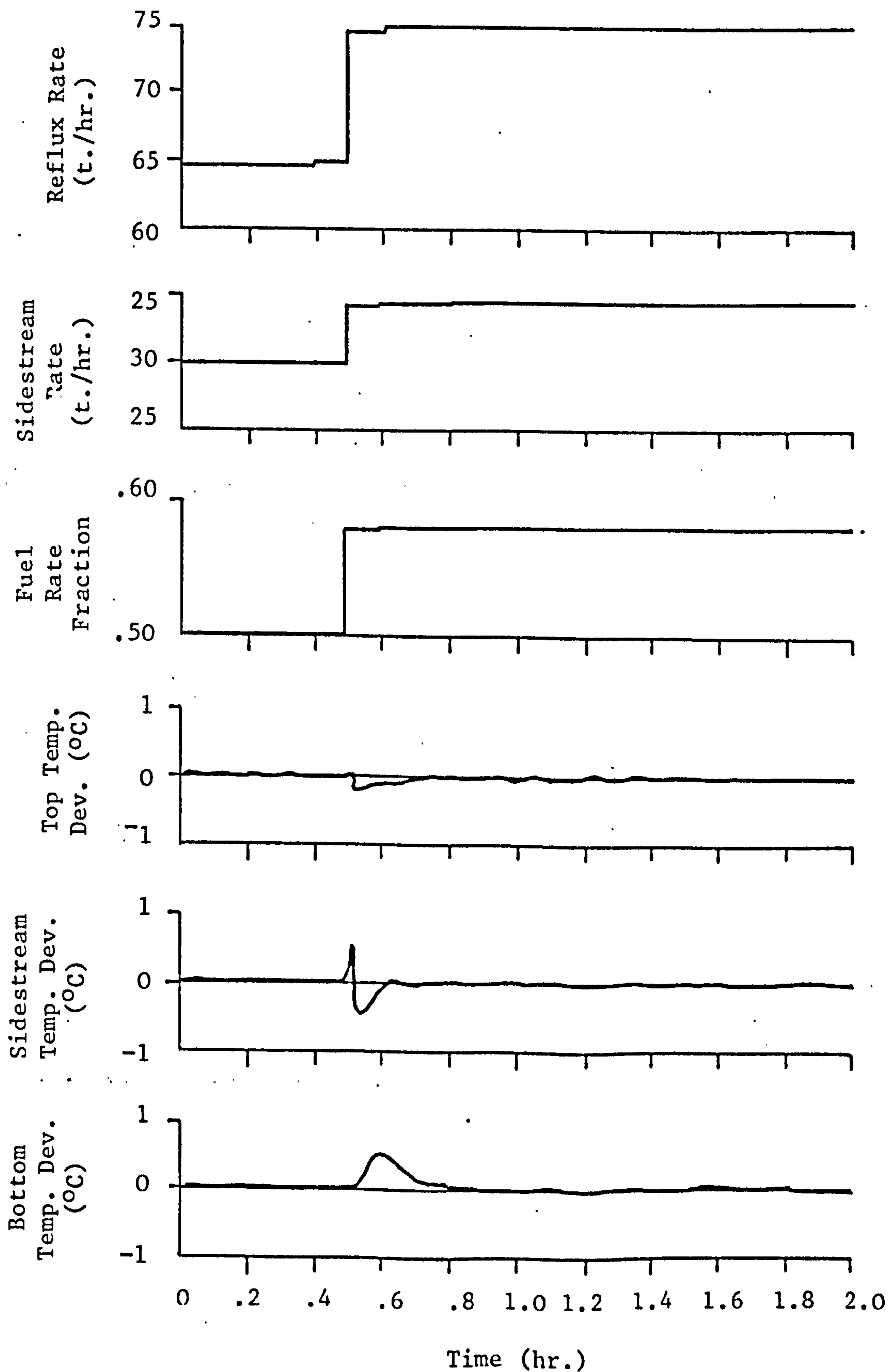


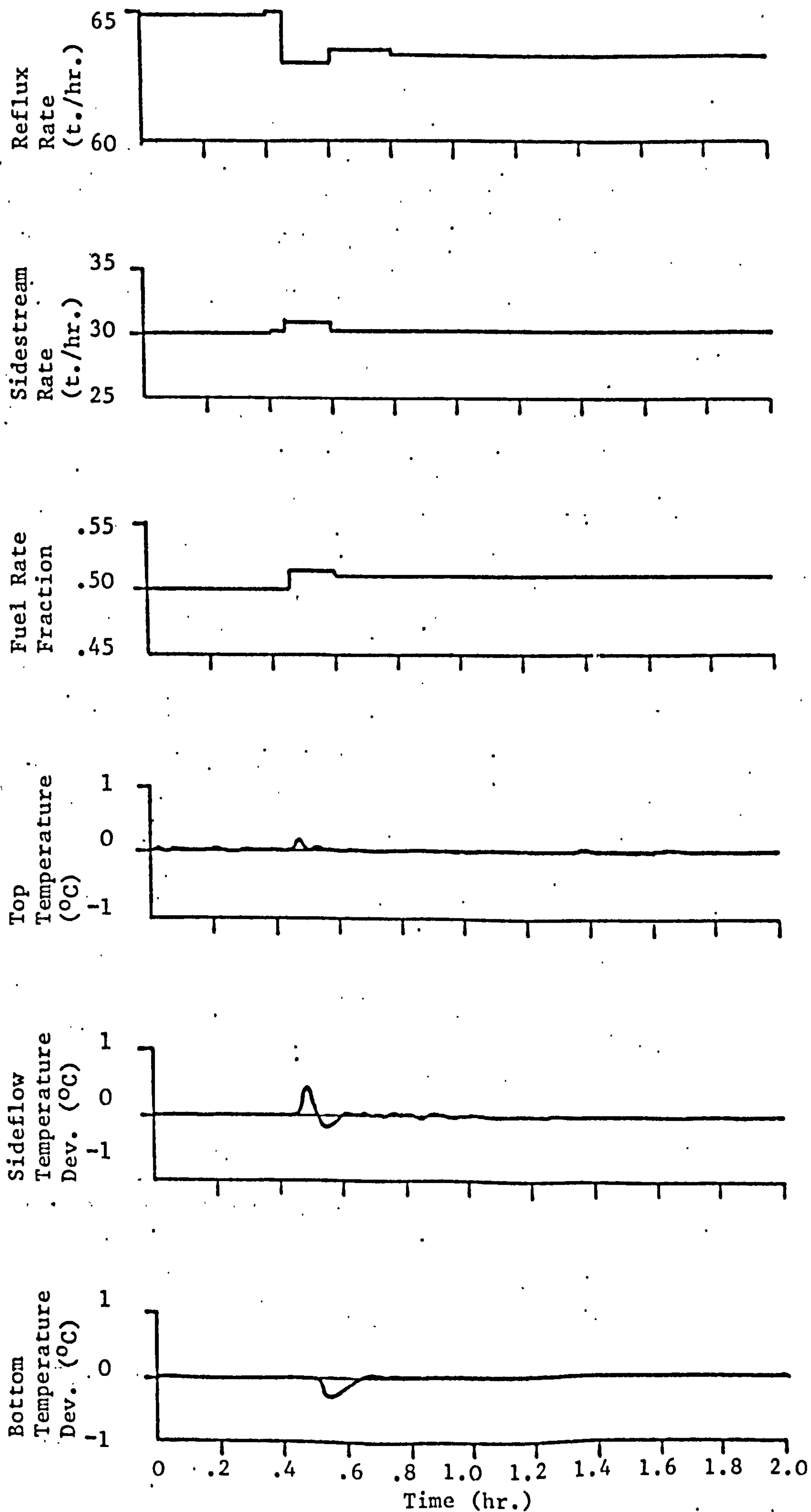
Figure 4.18 Splitter Regulatory Problem (Run SP2)Upsets: $T_F : 127.5^{\circ}\text{C} \rightarrow 117.5^{\circ}\text{C}$ at $t = .5$ hr. $I_{ss} = 2.03$ $I = .0159$ 

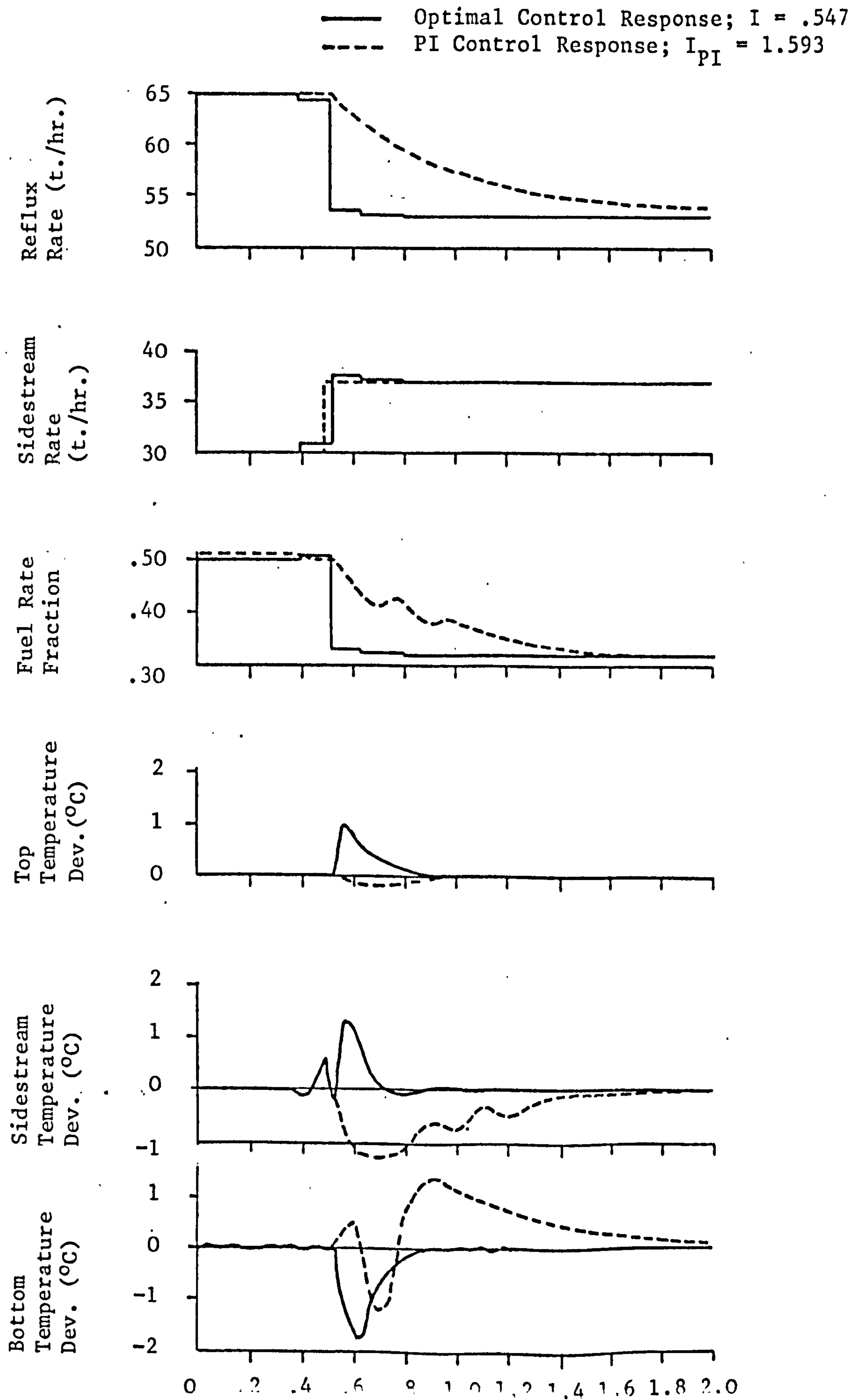
Figure 4.19 Splitter Regulatory Problem (Run SP3)Upsets: z_{F_1} : .30 $\rightarrow$.35 at $t = .5$ hr. z_{F_2} : .45 $\rightarrow$.425 at $t = .5$ hr. $I_{ss} = 1.361$ 

Figure 4.20 Splitter Servo Problem (Run SP4)

$$I_{ss} = 10.27$$

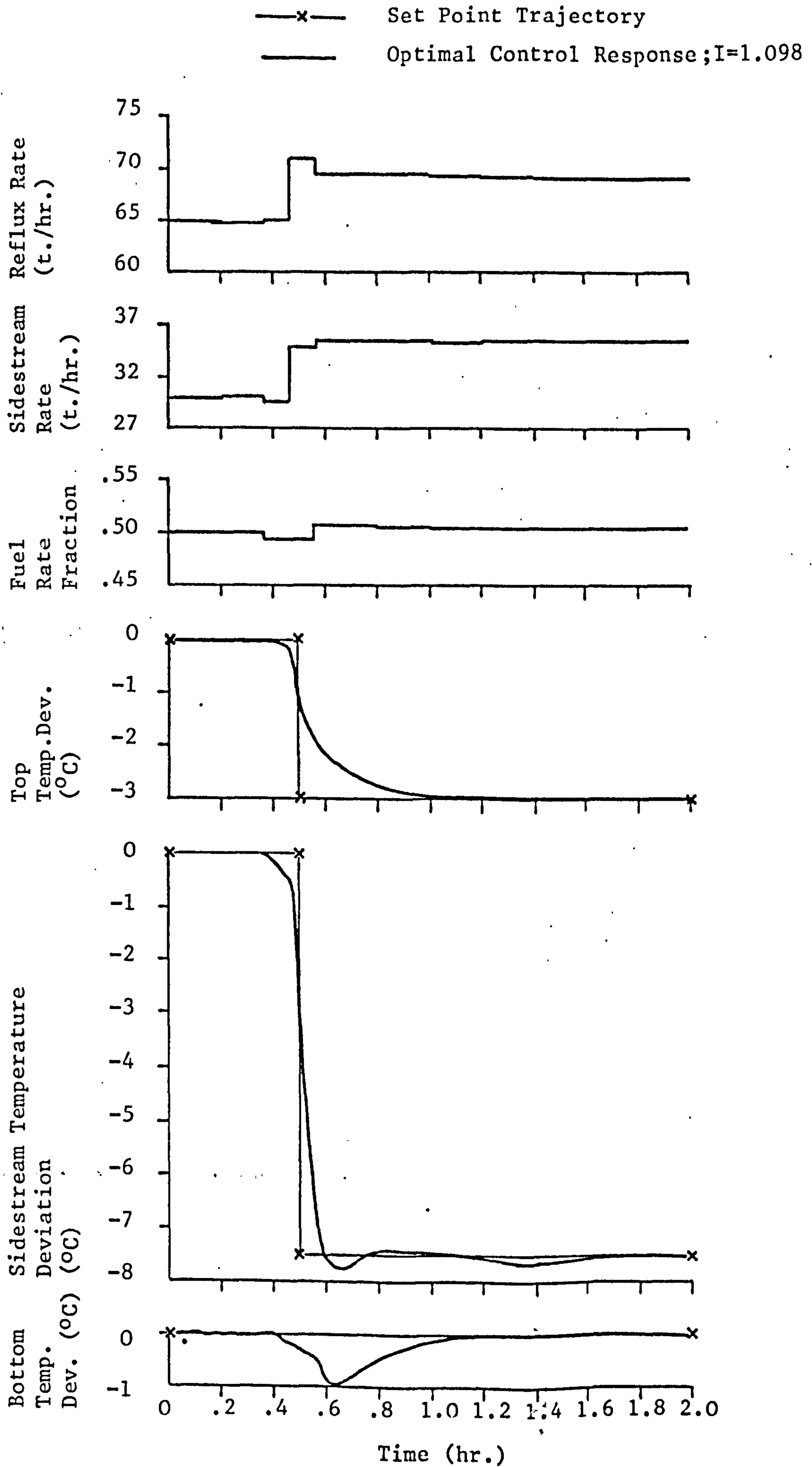
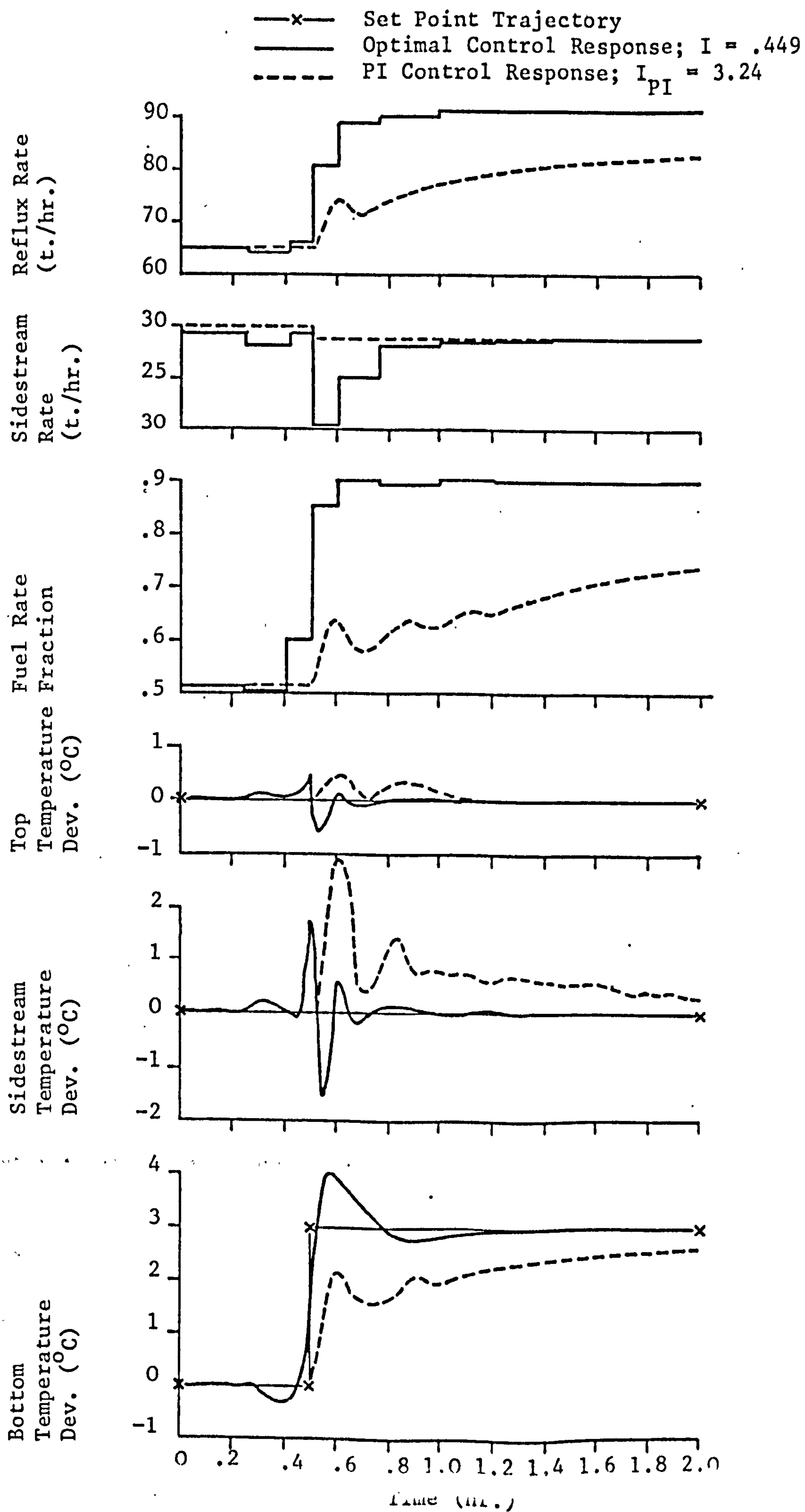


Figure 4.21 Splitter Servo Problem (Run SP5)

$$I_{ss} = 25.76$$



vaporization upsets affect the product streams very quickly, it is important that the state of the column be appropriate when the disturbance enters. The results confirm that considerable gains can be achieved through use of advance knowledge of upsets and final steady state control.

The effect of feed composition upsets on the product stream temperature is more lagged as demonstrated in Figure 4.19. Initial steady state controls are not changed until after the upset occurs at which point final steady state controls are approached via a fast first order lag. The response of a tuned P-I control system is also shown. The controller constants, supplied by BP were determined by trial and error, performing dynamic responses at various parameter settings until suitable trajectories were found. The control configuration was chosen with reflux and fuel rates controlling top and bottom temperatures respectively. Because of the high interaction between sidestream and distillate temperatures, no controller was used in conjunction with the sidestream; the flowrate was set to the final steady state at the upset. Because the controls are highly interactive, application of PI control results in an objective function value approximately three times that obtained using optimal control. The superiority of the optimal response is also reflected in the shorter time period necessary to re-establish steady state conditions.

The results of the servo problem are illustrated in Figure 4.20 and Figure 4.21. In Run SP4, the controls are changed before the prescribed set point switch in order that the transients may be centred about the switch time. Top and sidestream temperatures are decreased rapidly by implementing a reflux flow greater than its final steady state value in conjunction with a sidestream flowrate

slightly below the final steady state setting. This action is applied until the sidestream temperature is very close to its new set point. The high level of the reflux sends large amounts of cooler material down the column, thus causing a drop in the bottoms temperature. Recovery is managed through final steady state control, since higher fuel rates would disturb the top and sidestream temperatures.

The steady state trends for Run SP5, where the bottoms temperature is increased while the other temperature set points are maintained, have already been demonstrated as shown in Figure 4.16. From this figure, one would be tempted to control with only the reboiler heat load and reflux rate and leave the sidestream drawoff untouched. Figure 4.21 clearly reveals that this is not the optimal mode of operation, as the interaction between the reboiler heat load, reflux rate, and sidestream flowrate dominates the response characteristics. Before the prescribed set point change, all temperatures are raised by an increase in reboiler heating. The furnace heat and reflux rate are then drastically increased with the sidestream rate similarly decreased. At this point the sidestream temperature plummets, caused by the increased reflux action, but increases again because of the effect of the increased reboiler heating. Conversely the bottom temperature sharply rises due to the immediate effect of the fuel increase and overshoots its set point. However, the large amount of cooler material resulting from the increased reflux and decreased drawoff reaches the bottom of the column to force the temperature downward toward its set point. Steady state reflux and drawoff rates are then achieved via first order lags. This interactive control is much better than the sluggish PI

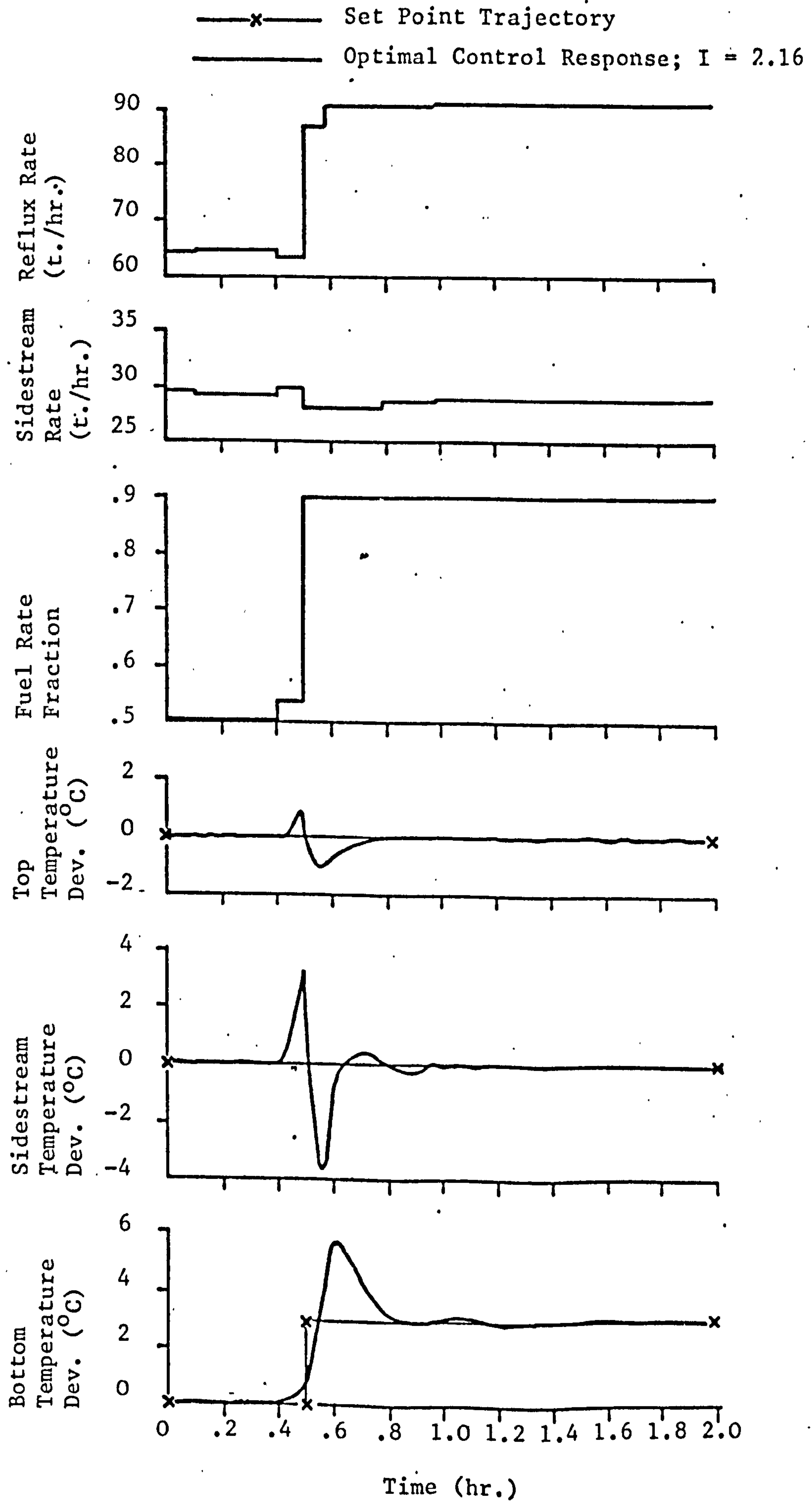
control system which hasn't even managed to obtain the new steady state at the final time.

Run SP5 clearly illustrates the advantage of utilizing all the degrees of freedom in the system even though some steady state values do not appreciably change. In an attempt to quantify this advantage, Run SP5 was repeated with the drawoff rate constrained to lie between 28.0 and 30.5 tonnes per hour. The results are shown in Figure 4.22. Because the lower bound on the sidestream rate is active for 0.28 hours, the set point offsets are much larger. The objective function value was 2.16 versus .449 for the previous case.

4.4 Summary

Optimal control responses of a refinery debutanizer were calculated for several types of problems, and these responses proved to be instructive when control structures were considered. It was found that standard feedforward/feedback systems for distillation columns could be implemented for regulatory purposes whereas a much more adventurous scheme can be employed for crude changeover problems. From the optimal responses, simple on-line policies were derived for both these control structures. For the difficult problem of facilitating set point changes which alter the degree of separation, the optimal control caused the entire contents of the column to move lighter together and heavier together.

For a splitter column, dynamic optimal control results were obtained for regulatory and servo problems. Knowledge of final steady state control proved valuable for the former problems whereas interactions between various controllers plays an important

Figure 4.22 Splitter Servo Problem (Run SP5)Sidestream Flowrate Constrained: $28 < S_2 < 30.5$ $I_{ss} = 25.76$ 

role in the latter. The implementation of conventional PI control resulted in more sluggish responses than those given by the optimal control.

CHAPTER 5 - DEVELOPMENT OF FEED CHANGEOVER POLICIES FOR

THE MAIN CRUDE COLUMN

5.1 Introduction

The fact that the main crude column processes from five to eight times the throughput of the debutanizer demonstrates the need for good changeover policies. Although the particular refinery of interest handles many crudes, these can be split into two groups (say group A and group B) representing two product spectrums. By far, the most difficult crude change is one corresponding to a group changeover, and this type will be taken as a basis for the studies presented here.

The splitter and debutanizer have been useful in illustrating the important aspects of changeover problems. The value of optimal set point switching policies developed in section 3.2.2 and implemented for a debutanizer servo problem in section 4.2.3 will become immediately apparent for the problems tackled in this chapter. Traditionally, control workers have designated a priori set point trajectories, usually by placing all importance on the final desired states from the start of the control period (Jarvis and Wright, 1972; Oakley and Edgar, 1976). This is valid for start-up or shut-down problems, but for changeovers where the initial specifications correspond to a viable operating condition, some set point switching policy is necessary. Both the previous studies have demonstrated the significance of steady state analysis in conjunction with dynamic optimization. For the main column, The British Petroleum Company Ltd. have supplied a steady state program that is capable of calculating column composition profiles for given flow, heating, and feed conditions.

All the optimal control problems solved in this chapter use the squared deviation from set point objective function discussed in section 3.3.1 . Final steady state control will be applied for the last control interval in order to avoid the final time constraint problems that were outlined in section 3.3.3. The ratio control concept which was introduced in section 3.3.3 to circumvent formulation of path constraints, will prove to be an asset in terms of control system structure. The results of the optimal control for the crude change are given in section 5.2. An analysis of the implementation aspects leads to two subproblems which are solved in sections 5.3 and 5.4.

Finally, the main column studies provide a test for the capability of OPCON to deal with large dynamic models which characterize many chemical engineering staged operations. Recently, Nishida et al. (1976) examined a twenty-state variable, seven-control variable, linear system and claimed that "this system seems to be one of the highest-order time optimal control problems that have ever been reported". The optimal control of the fifty-state variable, seven-control variable, non-linear, main column model should then represent a significant contribution to the chemical engineering control field.

5.2 Optimal Control of a Main Column Crude Changeover

The initial and final conditions for the crude changeover problem are shown in Table 5.1. This shift in operation is very dramatic as illustrated by the 25% decrease in the feed flowrate coupled with significant component concentration changes. The main column is preceded by a desalter drum which acts to delay feed composition upsets. Therefore, from the time a feed flowrate

TABLE 5.1 STEADY STATE CONDITIONS FOR CRUDE CHANGEOVER PROBLEM

Crude		A	B
F	(tonnes/hr)	470	360
z_{F1}		.17	.075
z_{F2}		.10	.075
z_{F3}		.10	.170
z_{F4}		.24	.380
z_{F5}		.39	.300
R	(tonnes/hr)	109.00	63.70
R_D		.44103	.42869
R_N		.11788	.00000
R_{KERO}		.14697	.08384
R_{LGO}		.39646	.53507
D	(tonnes/hr)	86.00	48.00
S_2	(tonnes/hr)	15.00	0.00
S_4	(tonnes/hr)	30.00	17.00
S_6	(tonnes/hr)	100.00	150.00
B	(tonnes/hr)	239.00	145.00
Q_3	(thermies/hr)	9103.70	10200.00
Q_6	(thermies/hr)	10400.00	9000.00
Q_9	(thermies/hr)	-1444.17	-1444.17
ϕ		.52	.62
y_{v1}^*		.7435	.4894
x_{22}^*		.4594	.2276
x_{43}^*		.3522	.4688
x_{64}^*		.3770	.4996
x_{95}^*		.6809	.5821

z_F - feed concentration

R_D - distillate ratio

R_N - drawoff ratio for S_2

R_{KERO} - drawoff ratio for S_4

R_{LGO} - drawoff ratio for S_6

ϕ - feed vaporization ratio

upset enters the system, all feed compositions are subjected to a first order lag with a time constant of .76 hours.

Optimal control calculations were performed using an objective function of the form:

$$I = \int_0^{t_f} \{ (y_{v1} - y_{v1}^*)^2 + (x_{22} - x_{22}^*)^2 + (x_{43} - x_{43}^*)^2 + (x_{64} - x_{64}^*)^2 + (x_{95} - x_{95}^*)^2 \} dt \quad (5.1)$$

where: y_{v1} is the concentration of component 1 in distillate stream, D, shown in Fig. 3.5(b), x_{ij} is the concentration of the j th component in the i th column section, and superscript * denotes set point.

A value for t_f of 7 hours was selected with final steady state control applied for at least the final 3 hours, (i.e. upper limit for final switching time set at $t = 4$ hours). This was considered to be reasonable since preliminary simulations revealed that application of final steady state control resulted in a dynamic period of approximately 4 hours. The number of control intervals, NCI, was chosen to be 10. Since the optimal set point switching policy is incorporated into the optimal control calculations, the initial control value cannot be selected as those to maintain the instantaneous set points, as was the case for the splitter and some debutanizer runs. The controls were initially switched to final steady state control at the time of the flowrate upset with the set points chosen according to the optimal switching policy.

Limit values for the control variables are shown in Table 5.2. The upper bound on the distillate ratio ensures that sufficient reflux will be available. The sidestreamdrawoff ratios have upper limits to prevent the column running dry; these limits depend upon

TABLE 5.2 CONTROL VARIABLE BOUNDS

Variable	Lower Bound	Upper Bound
R_D	0	0.8
R_N	0	0.4
R_{KERO}	0	0.5
R_{LGO}	0	0.6
Q_3	3000	12000
Q_6	5500	15000
ϕ	0.40	0.65

drawoff location since the problem becomes less critical towards the bottom. Lower bounds on the heating loads of the recirculating refluxes are necessary because these streams are utilized to reboil other columns. Minimum and maximum furnace heating loads were transformed into the bounds on the feed vaporization ratio. Since this ratio depends upon the physical properties of the feed, the values shown in Table 5.2 represent an average of the two feeds.

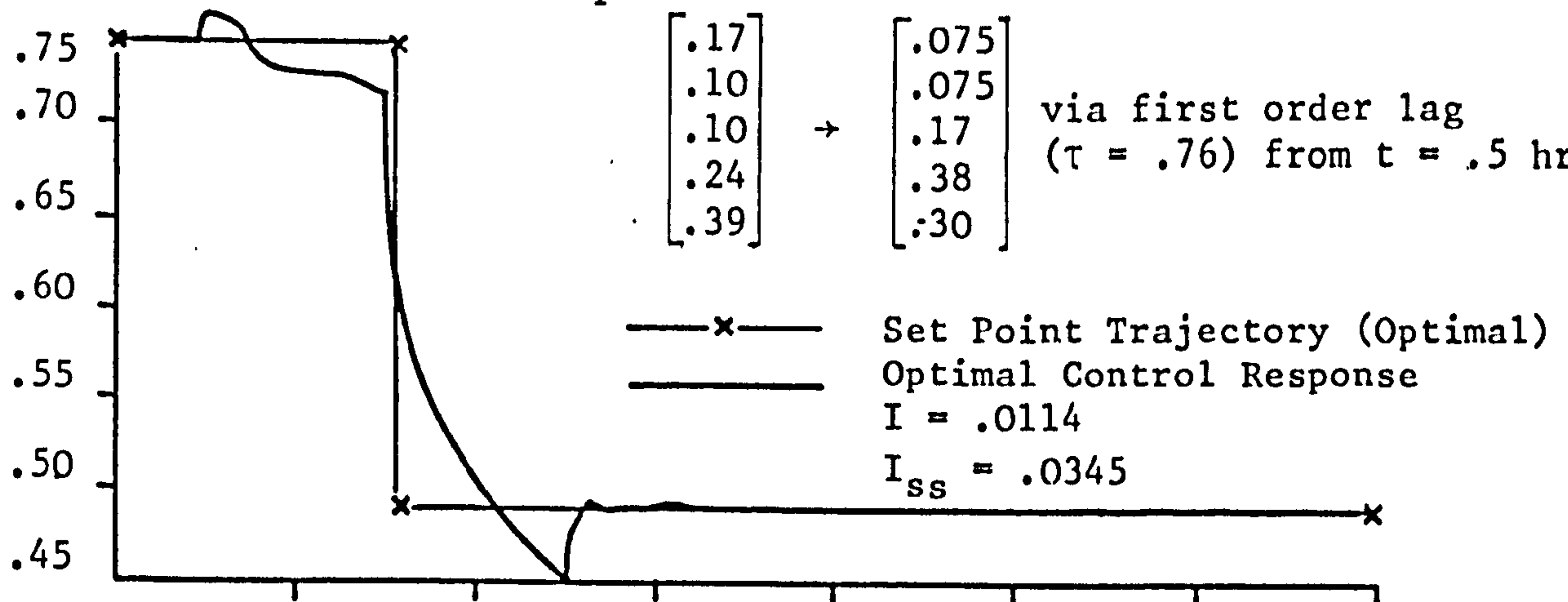
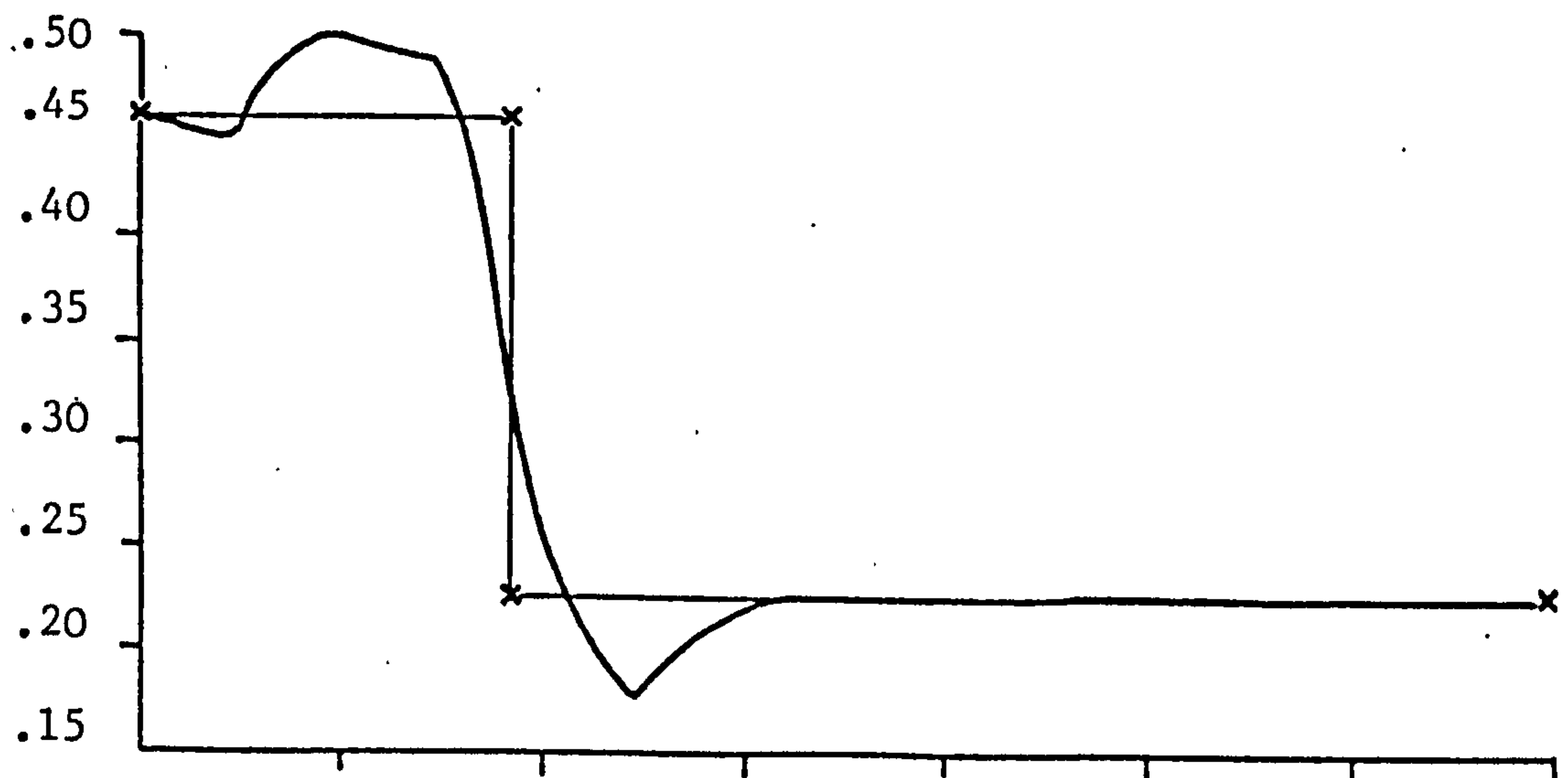
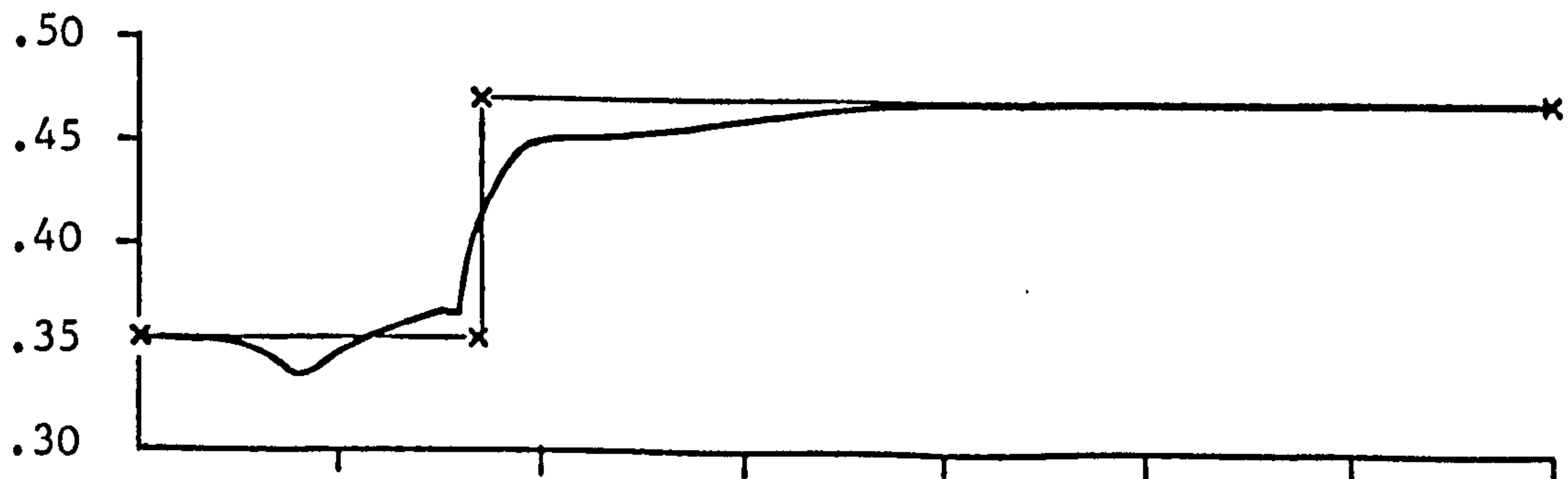
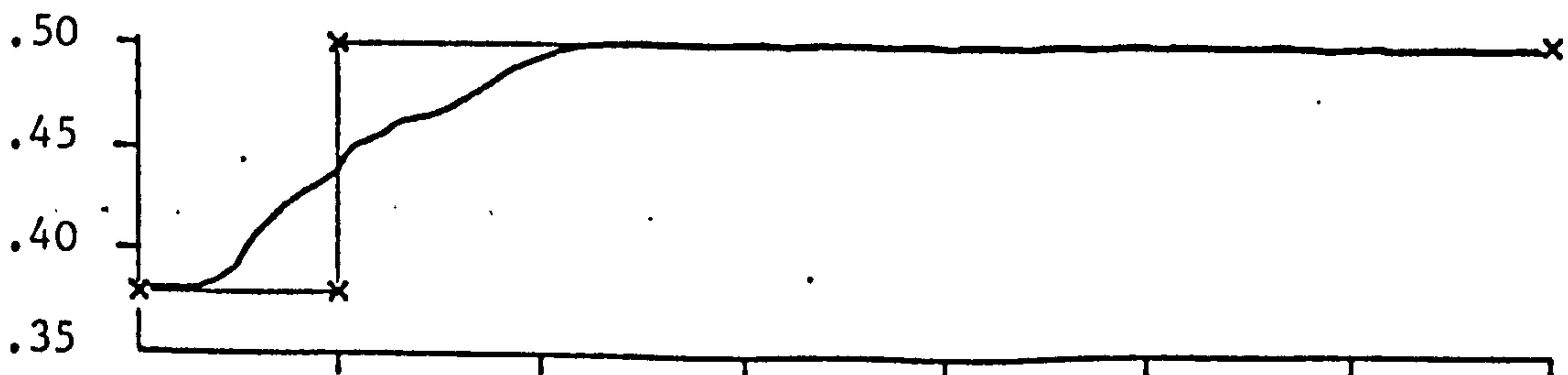
Coding and verification of the dynamic main column model for input to OPCON was performed in a manner similar to that outlined for the splitter in section 4.3.2. Results of the dynamic optimization are shown in Fig. 5.1 - 5.3. The optimal flowrate controls in Fig. 5.2 represent the drawoff rate rather than the piecewise constant drawoff ratio. Also, the upper and lower reflux heating rates in Fig. 5.3 are expressed as ratios with respect to the upper limit values given in Table 5.2.

The optimal control reduced the steady state control objective function by a factor of three from .0345 to .0114. For practical purposes, the new set points are achieved approximately 2.5 hours after the flowrate upset. This time represents 3.3 times constants of the feed composition input trajectory thus demonstrating the feed-forward nature of the controls; knowledge of the disturbances and new set points allowed attainment of the new steady state just after the full effect of the composition changes reached the entrance of the column.

Examination of Fig. 5.2 and 5.3 reveal that product stream flowrates are much more active than heating controls during the changeover period. The latter do little more than move to the new steady state values. The gradual drop in the distillate rate from

Figure 5.1 Optimal Concentration Responses For Crude ChangeoverProblemUpsets: F: 470 t./hr. $\rightarrow$ 360 t./hr. at $t = .5$ hr. z_F :

$$\begin{bmatrix} .17 \\ .10 \\ .10 \\ .24 \\ .39 \end{bmatrix} \rightarrow \begin{bmatrix} .075 \\ .075 \\ .17 \\ .38 \\ .30 \end{bmatrix}$$

via first order lag
($\tau = .76$) from $t = .5$ hr. y_{v1}  x_{22}  x_{43}  x_{64}  x_{95} 

Time (hr.)

Figure 5.2 Optimal Flowrate Controls For
Crude Changeover Problem

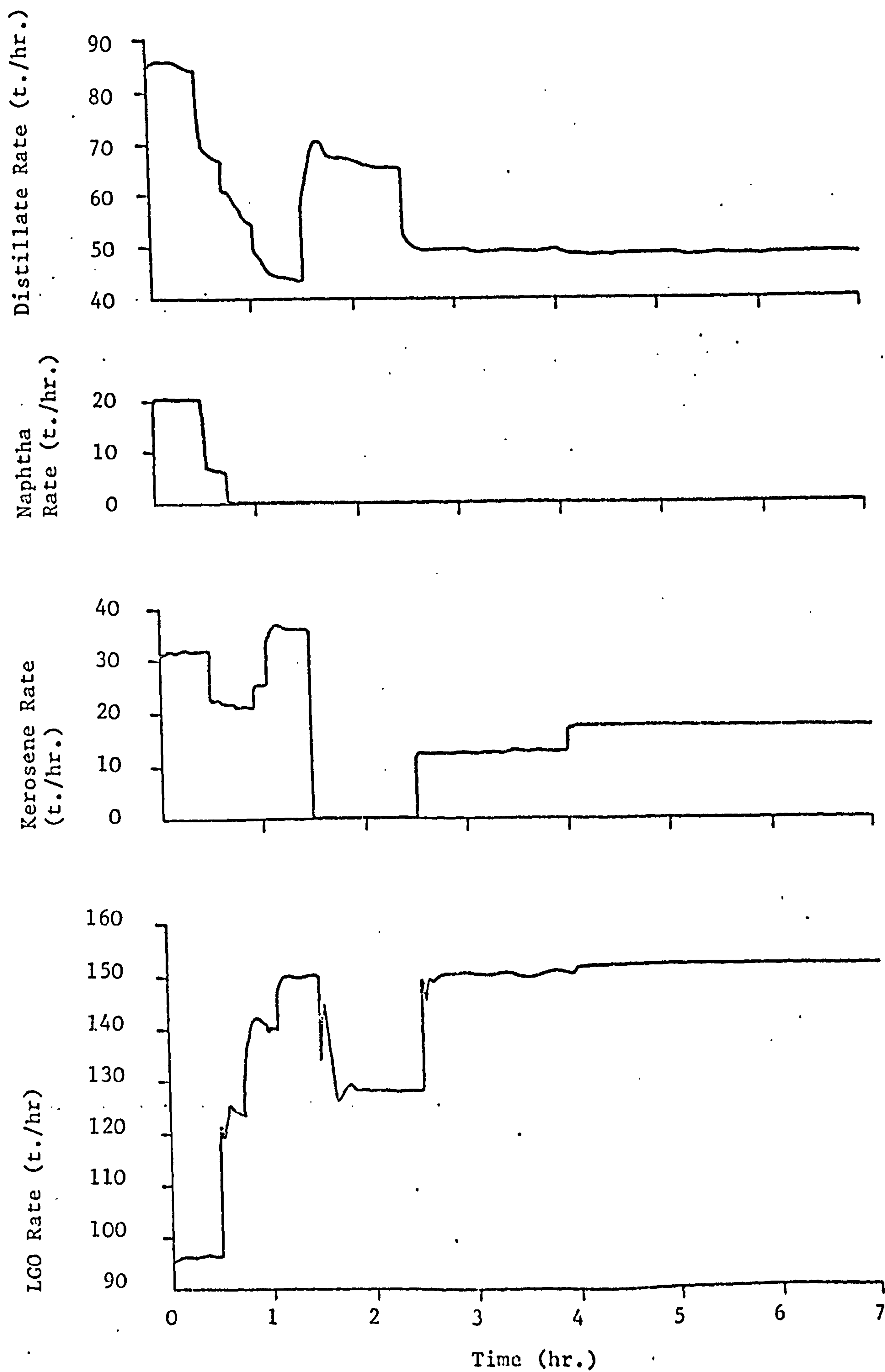
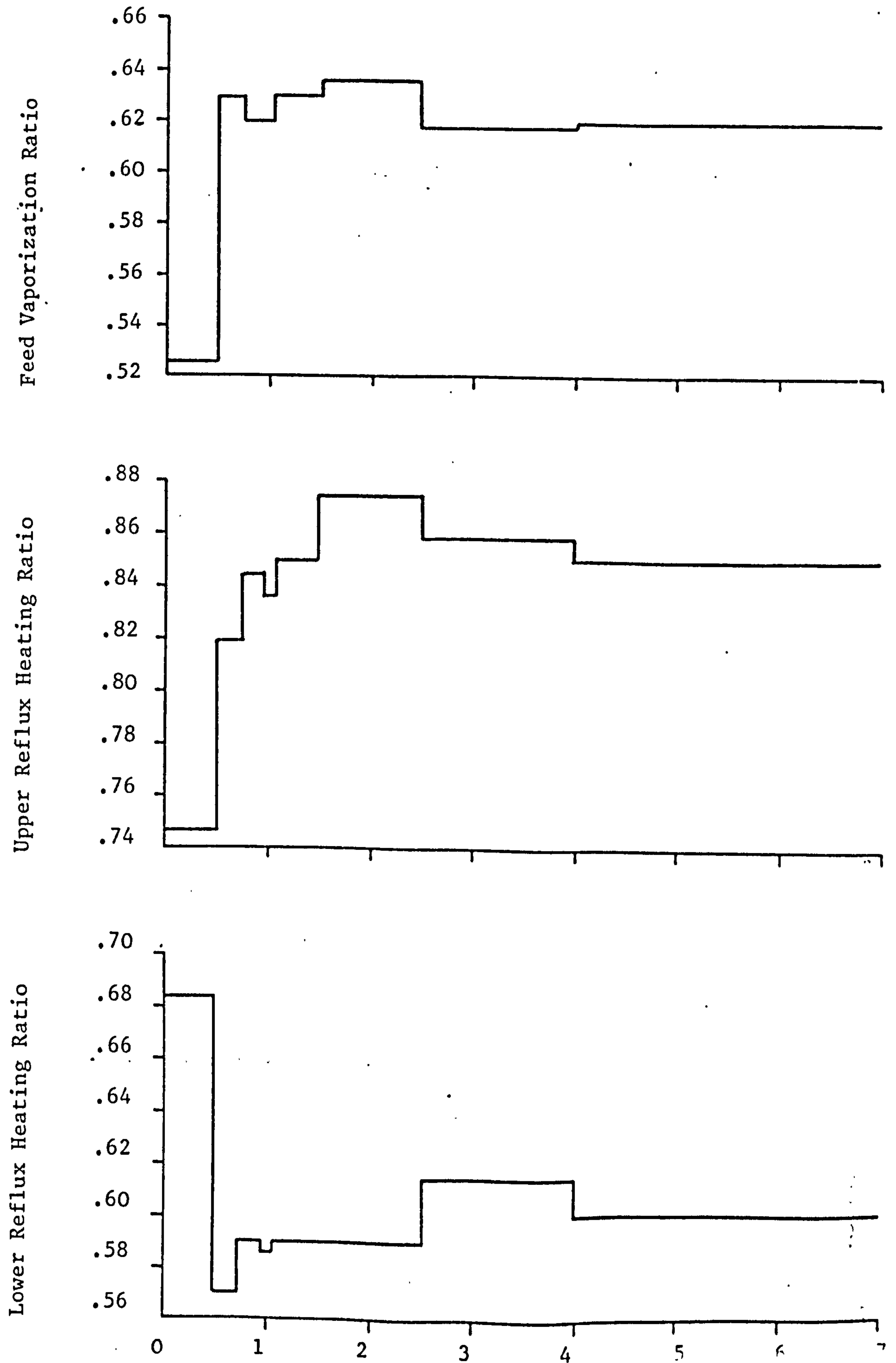


Figure 5.3 Optimal Heating Controls For
Crude Changeover Problem



the time of the feed flow upset maintains the top set point specification. At $t = 1.5$ hr., the large increase in the distillate rate and corresponding decrease in the reflux flow, through the reflux drum level controller, effect rapid decreases in top two product key components. At the same time, the kerosene rate is dropped to zero which promotes a rapid change in the key component towards the new set point. The increased flow of middle components down the column resulting from decreases in the kerosene and light gas oil rates causes the heavy component in the residue to decrease sharply. Since the light gas oil drawoff is close to the feed location, the effect of feed concentration changes are more immediate than for the drawoffs further up the column. For this reason, the initial set point is difficult to maintain, and the changeover of its key component occurs slowly in comparison with the other product streams. Note that the key component responses for the distillate, naphtha, and residue streams overshoot their new set points, but these are reestablished as the effect of the new feed composition reaches the column extremes.

Apart from the light gas oil stream, the optimal control maintains the original set points for one hour after the feed flowrate upset. In terms of implementation, a strategy could be devised whereby feedback control, based on the initial specifications, would be utilised until this point, when the process set points would be changed on the controllers. However, this would not ensure the fast responses which characterized the optimal changeover. Perhaps a better approach is evident from the splitter studies. It was shown that feed flowrate

upsets are transmitted through the column very quickly in comparison with feed composition upsets. If the light gas oil stream is neglected because of its close proximity to the feed plate, it can be stated that the initial set points were maintained until the effects of the flowrate upset were overcome. Two subproblems can then be postulated in which the feed rate of crude A is changed to match that of crude B without alteration of initial product specifications, followed by the required feed composition changeover. In this manner, the fast effects associated with the feed flowrate change can be separated from the slower response to the feed composition change.

The evolution of these two subproblems could not automatically arise from the original problem formulation. Feed flowrate was not selected as a control variable because of its heavy interaction with the rest of the plant, especially through the feed preheat train. However, movement of the time position of step change in feed flow, with respect to the feed composition upset, is not likely to create any practical difficulties. Compensation for loss in capacity of the column for the short period of time between the feed flow and composition change will occur during the reverse changeover problem.

5.3 Subproblem (i) - Optimal Feed Composition Changeover Policies

Subproblem (i) represents the second phase of control suggested by the previous results. The object is to switch the set points in face of a feed composition change only; it is assumed that the feed flowrate change has already been undertaken. The type of feed composition delay will be the same as used in the

main problem (i.e. first order lag, $\tau = 0.76$) starting from $t = 0.5$ hr. Objective function and optimal control parameters are identical to those outlined in section 5.2.

The initial and final conditions for subproblem (i) are shown in Table 5.3. Note that the steady state set points of crude A_1 do not correspond exactly to those of crude A shown in Table 5.1 of section 5.2. Under normal circumstances, heating rates and product drawoffs would be scaled with the ratio of the two feedrates to ensure equivalence of these set points. However, since the bottoms heating rate, $-Q_9$, is constrained to be the same for both crudes A and B, this is not possible. A steady state program could be written to determine controls to maintain the set points, but because this is a one-off exercise, a more practical approach would be to adjust the controls on the BP supplied program until approximate agreement is found. The steady state conditions for crude A_1 represents application of this approach. The small discrepancies in the set point values between crudes A and A_1 are not considered serious since they are not expected to alter the trends of the optimal responses.

The optimal results are presented in Fig. 5.4-5.6. The optimal controls led to an objective function of .00897 compared with .03305 for application of steady state control. As expected, the optimal controls for this subproblem yielded better performance than those for the main problem as is evident from the faster response trajectories and consequently lower objective function value. Examination of Fig. 5.5 and 5.6 reveals that, apart from the feed vaporization ratio, flowrate controls are much more active than heating controls. The significance of the feed vaporization ratio achieving its upper limit will be discussed

TABLE 5.3 STEADY STATE CONDITIONS FOR CRUDE CHANGEOVER

SUBPROBLEM (i)

Crude		A ₁	B
F	(tonnes/hr.)	360	360
z_{F1}		.170	.075
z_{F2}		.100	.075
z_{F3}		.100	.170
z_{F4}		.240	.380
z_{F5}		.390	.300
R	(tonnes/hr.)	70.00	63.70
R_D		.48905	.42869
R_N		.12306	.00000
R_{KERO}		.11807	.08384
R_{LGO}		.46502	.53507
D	(tonnes/hr.)	67.0	48.00
S ₂	(tonnes/hr.)	10.0	0.00
S ₄	(tonnes/hr.)	18.0	17.00
S ₆	(tonnes/hr.)	96.0	150.00
B	(tonnes/hr.)	169.0	145.0
Q ₃	(thermies/hr.)	8000.0	10200.00
Q ₆	(thermies/hr.)	9000.0	9000.0
Q ₉	(thermies/hr.)	-1444.47	-1444.47
ϕ		.52	.62
y_{v1}^*		.7321	.4894
x_{22}^*		.4485	.2276
x_{43}^*		.3433	.4688
x_{64}^*		.3691	.4996
x_{95}^*		.7012	.5821

 z_F - feed concentration R_D - distillate ratio R_N - drawoff ratio for S₂ R_{KERO} - drawoff ratio for S₄ R_{LGO} - drawoff ratio for S₆ ϕ - feed vaporization ratio

Figure 5.4 Optimal Concentration Responses For
Crude Change Subproblem (i)

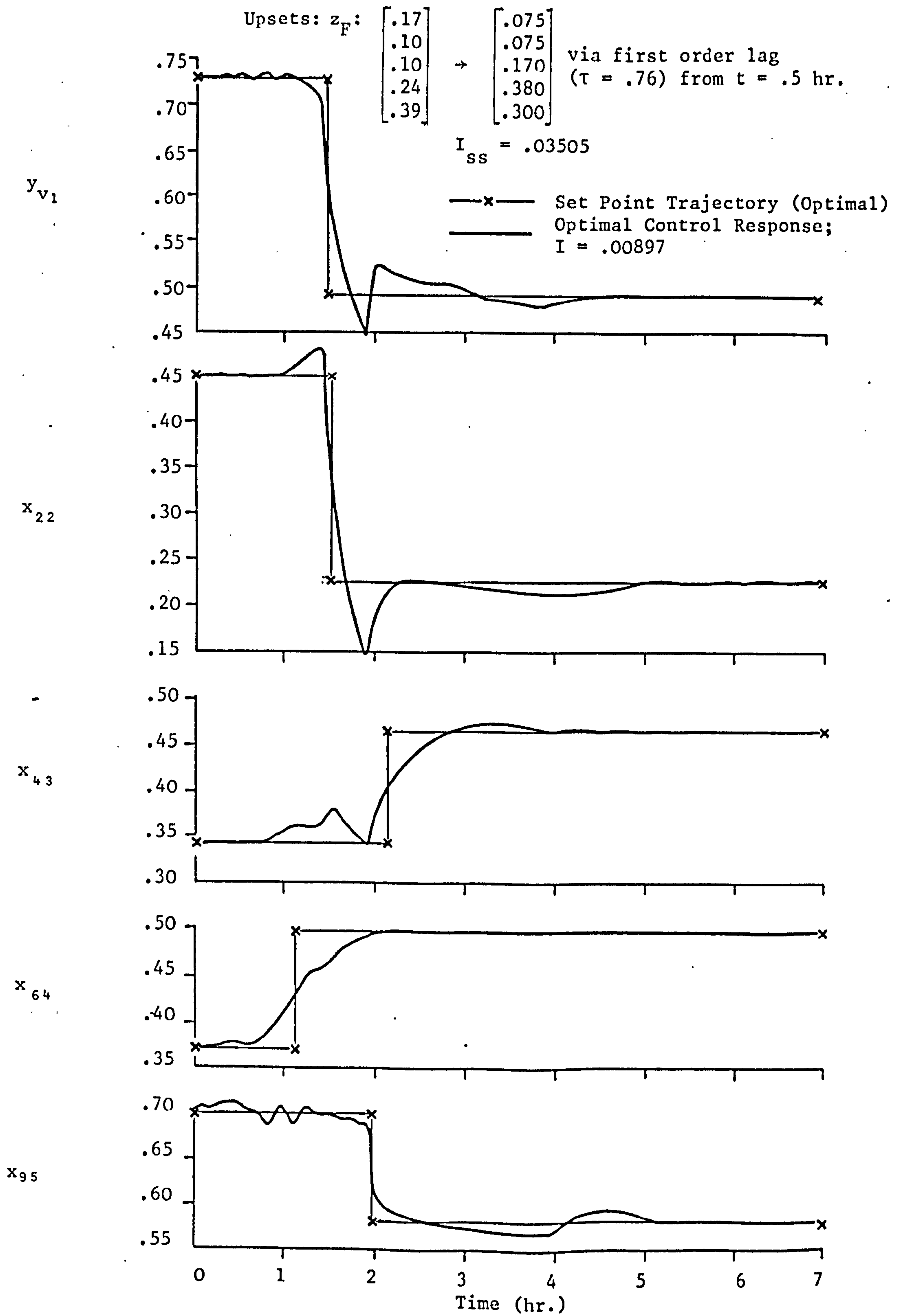


Figure 5.5 Optimal Flowrate Controls For
Crude Change Subproblem (i)

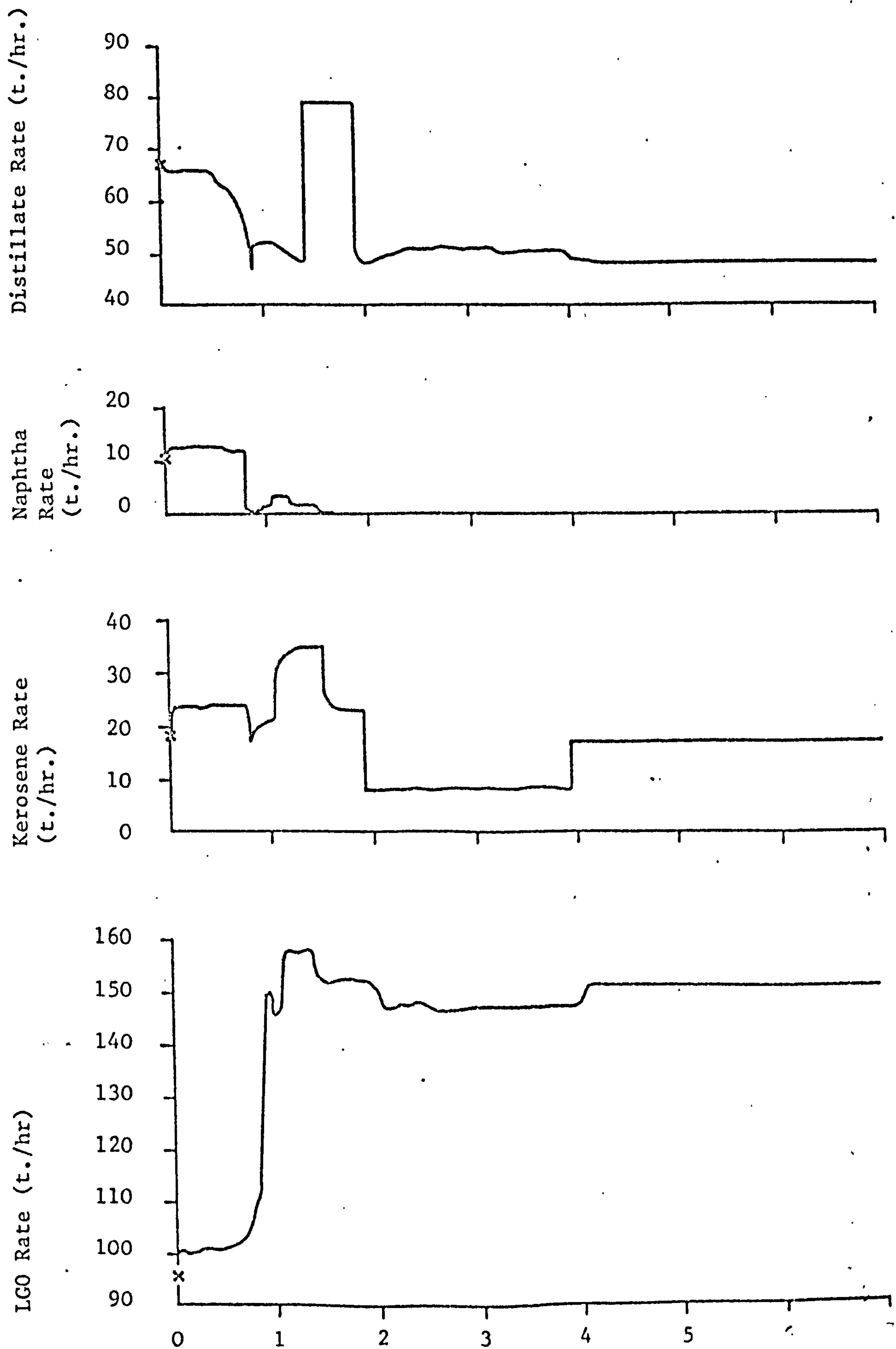
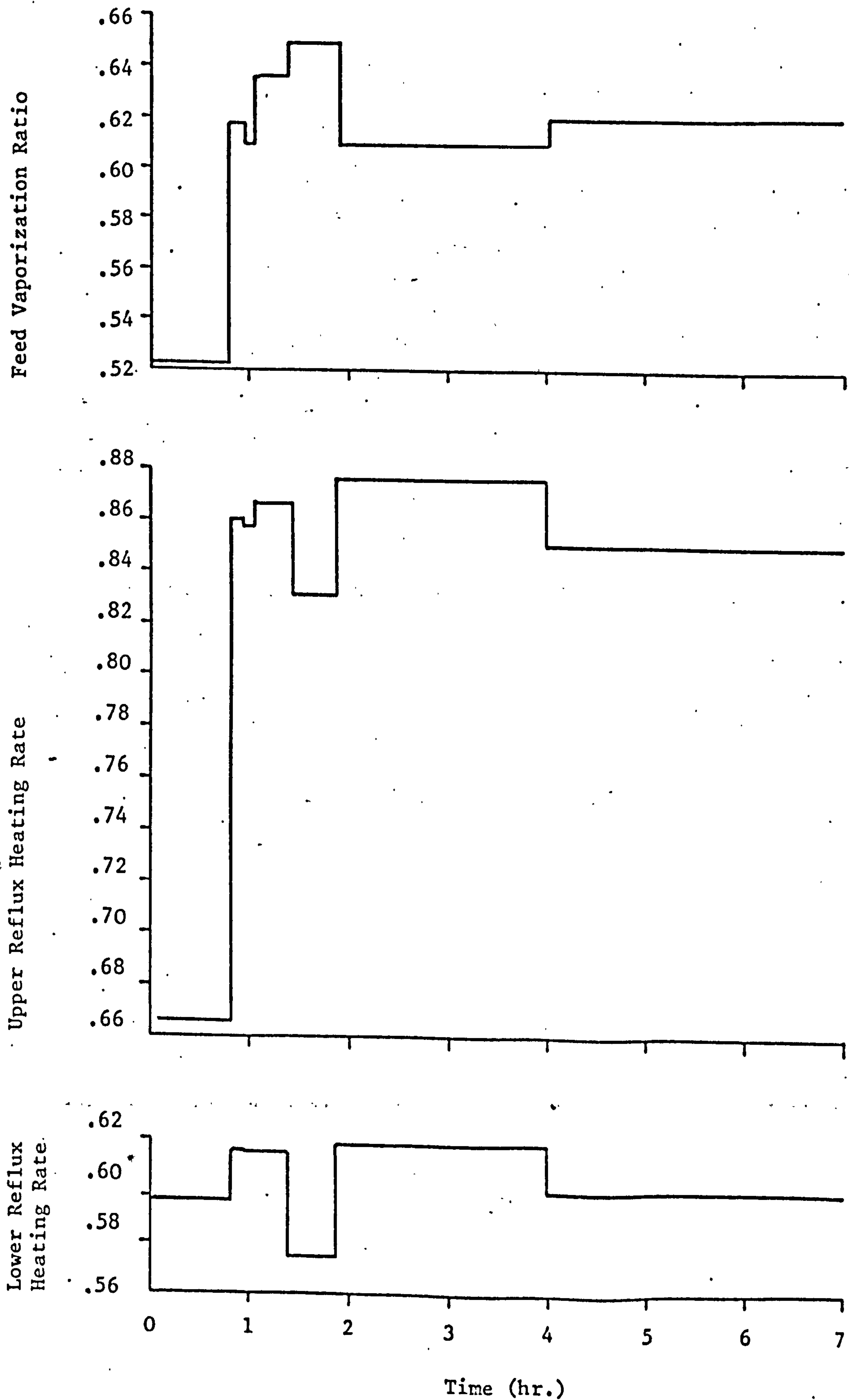


Figure 5.6 Optimal Heating Controls For
Crude Change Subproblem (i)



later.

The prominent feature of the concentration responses is that, the column contents move heavy together and then light together. Specifications of the kerosene and residue streams were maintained while distillate and naphtha streams underwent set point changes and overshoot their new specifications. These were re-established while the kerosene and residue streams were driven to their new set points. This trend is the same as that observed for the debutanizer servo problem in section 4.1.3. Note that all products attain new specifications by 2.5 hours after the start of the feed composition upset.

Analysis of control trajectories which facilitated these specification changes indicates the possibility of some sub-optimal control structures. The major switch for the liquid drawoff and heating rates occurred at 0.8 hours. This switch on the LGO rate serves to drop the residue rate through the reboiler level control system which maintains the bottom set point even though the new feed contains less of the heavy component. In the same manner, it appears that kerosene drawoff rate is used to control the kerosene key component at its initial specification for the first two hours of operation. The very fast set point changes for the distillate and naphtha products are effected by two simultaneous control actions: the feed vaporization ratio is increased to its upper bound ($\phi = 0.65$) together with a large increase in the distillate drawoff. This causes a large amount of light component to be driven out of the column through the distillate and naphtha streams, and this extreme control action is not terminated until key component responses of both products have overshoot their new specifications. At this point, the kerosene drawoff is lowered

to facilitate the kerosene key component changeover, and the feed vaporization is dropped to create the heavy component changeover of the residue. Meanwhile, placement of the feed vaporization and distillate rate to final steady values together with the effect of feed composition changes cause the key components of the top two product streams to return to their new specifications.

5.3.1 Implementation Aspects

Now that optimal results are available and have been rationalized, the problem of developing simple on-line policies can be examined. A series of simulations will be performed that extract the dominant features of the optimal responses yet allow for the practicalities associated with implementation. The worthiness of any sub-optimal control trajectory can be quantified in terms of the optimality approach factor, OAF, defined by Eq.(4.7) in section 4.1.3 for the debutanizer study. A summary of all sub-optimal runs is provided in Table 5.4 and the runs presented there will be discussed in turn.

Runs 1, 2 and 3

Upper and lower bounds on OAF are established through application of optimal and steady state control respectively. It should be noted that, although steady state control is represented by zero value of OAF, this control would probably outperform conventional feedback control as demonstrated in some of the splitter runs. Certainly, in this highly interactive system, single loop control would not be expected to yield good system responses. From the optimal control trajectories in Fig. 5.5 and 5.6, the major control

TABLE 5.4 SUMMARY OF SUB-OPTIMAL CONTROL POLICIES FOR CRUDE CHANGE SUBPROBLEM (1)

Run	Description	I	OAF
1	Steady state control; switch .5 hr	.03305	0.000
2	Optimal control	.00897	1.000
3	Steady state control; switch .79 hr	.03271	.0141
4	Steady state control; switch .79 hr		
a	$\{\phi = .65, R_D = .5\}$; 1.4 $\rightarrow$ 1.8 hr	.02095	.5024
b	$\{\phi = .65, R_D = .5\}$; 1.4 $\rightarrow$ 1.9 hr	.01738	.6507
c	$\{\phi = .65, R_D = .55\}$; 1.4 $\rightarrow$ 1.9 hr	.01388	.7960
d	$\{\phi = .65, R_D = .60\}$; 1.4 $\rightarrow$ 1.9 hr	.01617	.7010
e	$\{\phi = .65, R_D = .60\}$; 1.4 $\rightarrow$ 1.8 hr	.01445	.7742
f	$\{\phi = .65, R_D = .60\}$; 1.4 $\rightarrow$ 1.7 hr	.01557	.7259
5	Steady state control; switch .79 hr		
	$\{\phi = .65, R_D = .55\}$; 1.4 $\rightarrow$ 1.9 hr; $R_{KERO} = .2$, 1.0 $\rightarrow$ 1.4 hr	.01353	.8106
6	Steady state control; switch, Q_3 , .79 hr; others, .87 hr		
	$\{\phi = .65, R_D = .55\}$; 1.4 $\rightarrow$ 1.9 hr; $R_{KERO} = .2$, 1.0 $\rightarrow$ 1.4 hr	.01320	.8243
7	Steady state control; switch, Q_3 , .79 hr; others, .87 hr		
	$\{\phi = .65, R_D\}$ ($y_{v_1} = .675$) $\rightarrow$ ($y_{v_1} = .450$)		
a	$R_D = .42869$	.02562	.3085
b	$R_D = .45$	.02082	.5079
c	$R_D = .50$	.01543	.7317
d	$R_D = .55$	.01415	.7849
e	$R_D = .60$	.01712	.6615
f	$R_D = .65$	.02495	.3363
8	Same as 7d) except:		
	$R_{KERO} = .11807 + K_{KERO}(x_{43} - .3433)$; $t = 0 \rightarrow (y_{v_1} = .450)$		
a	$K_{KERO} = 2$	.01329	.8206
b	$K_{KERO} = 1$	.01313	.8272
9	Same as 8b) except:		
	$R_{LGO} = .46502 + K_{LGO}(x_{95} - .7012)$; $t = 0 \rightarrow (y_{v_1} = .450)$		
a	$K_{LGO} = 1$	.01304	.8309
b	$K_{LGO} = 5$	.01260	.8492
c	$K_{LGO} = 10$	.01260	.8492

switch occurs sometime after the feed composition upset thus providing incentive to explore simple policies based on switches between the steady state controls. However, Run 3, which was performed with the steady state switch at $t = .79$ hours, illustrates that this leads to little significant improvement over switching at $t = 0.5$ hours.

Runs 4, 5 and 6

A very important part of the optimal responses was fast changeover of the top product streams effected by large increases in the feed vaporization and distillate drawoff ratios. This extreme control action was not applied until 0.9 hours after the upset since combination of the new steady state control with the delayed effects of feed changes through the column maintained the original top product specification. Clearly, response performance is a function of both the level of extreme action and timing of its application. For the optimal response, the feed vaporization, ϕ , reached its upper bound and this should be imposed for the sub-optimal strategies. The problem still remains of choosing distillate drawoff ratios together with application times and this is investigated in Run 4. The optimal control response gave $R_D = .55$ for 0.5 hours at the optimum and this is validated in Run 4c). However, similar performance is achieved by using $R_D = .60$ for 0.4 hours. Such trends make physical sense: a higher level of extreme control implies a faster response and thus a shorter period of application is required. However, it is clear that the largest possible R_D value should not be used in that it must remain consistent with ϕ which has been set to its upper bound. The benefit derived from application of this type of policy is large

as evident from OAF values up to .7960.

From Fig. 5.5, it can be seen that the kerosene drawoff does not move directly towards its new steady state value at $t = .79$ hr, but rather moves to maintain the key component at its set point. Run 5 is performed using the conditions of Run 4d) except R_{KERO} is set to .2 from 1.02 to 1.39 hours, which results in a slight improvement of the OAF value to .8106. Run 6 stems from a practical consideration. There is a large increase in the LGO drawoff rate at the steady state switch, and under normal circumstances the extra material is provided by the increased cooling rate of the upper recirculating reflux. However, if these controls are switched at the same time, the undersirable situation may arise whereby more material is withdrawn than available because increased internal liquid rate created by the increased cooling does not immediately reach the drawoff location. In order to circumvent this possible difficulty, Run 6 was devised which used the same conditions as Run 5 except that the upper recirculating reflux was switched at 0.79 hr. and all other controls switched at 0.87 hr. Although negative internal liquid flowrates never actually occurred in Run 5, a minimum value of 4.8 tonnes/hr. was observed just after the switch, and this minimum was increased to 10.3 tonnes/hr. in Run 6, without reduction of the OAF.

Runs 7, 8 and 9

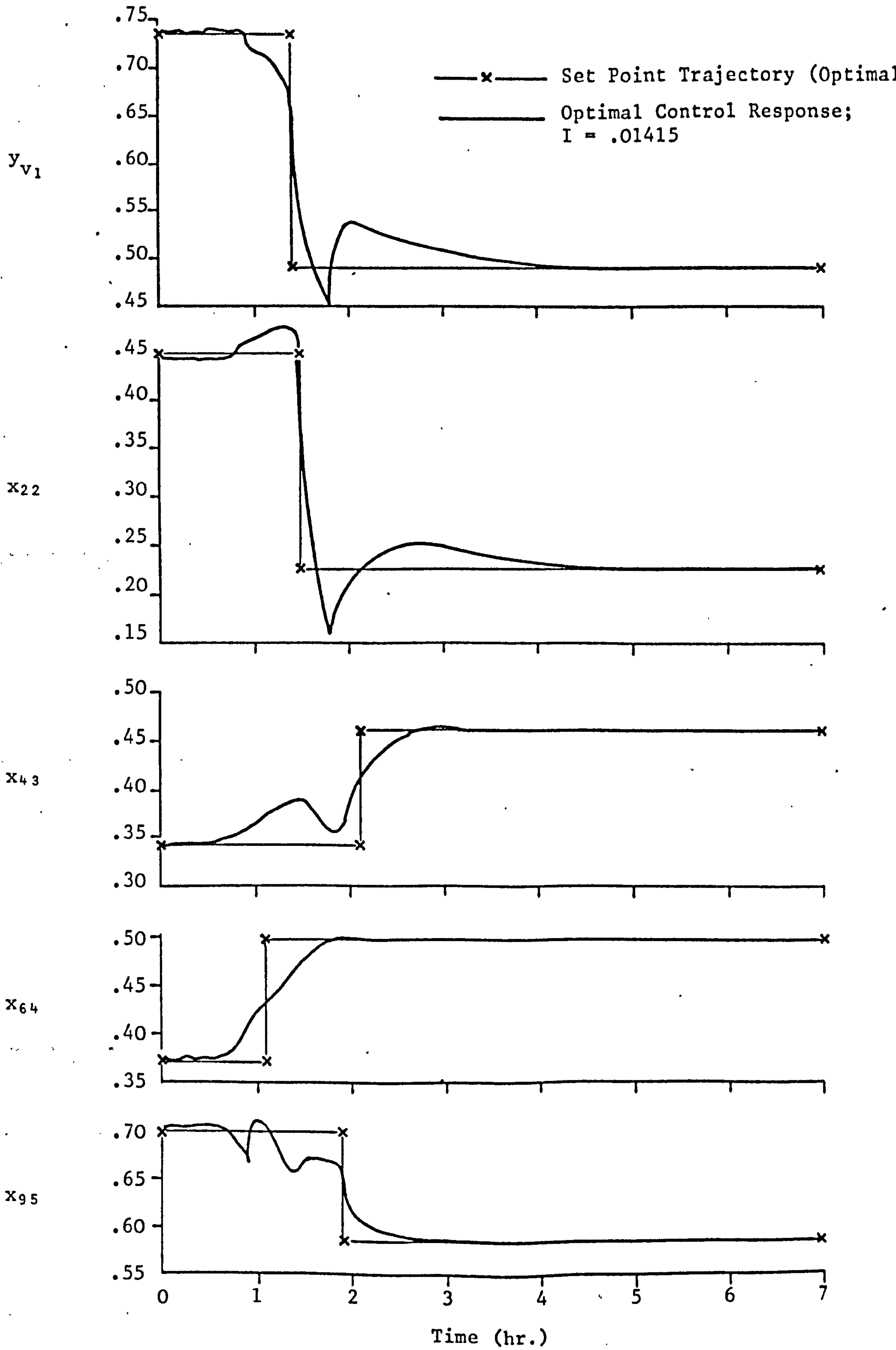
The previous runs have been concerned with attempts at duplicating the optimal responses using simple open-loop sub-optimal policies. It is of practical interest to seek some feedback that would allow an on-line system to counteract modelling inaccuracies. Some insight along these lines can be gained from the debutanizer

studies. An on-line switching rule was derived which signalled the termination of extreme control action. Examination of Fig. 5.4 yields the condition of y_{v_1} as a similar switching rule and this possesses the distinct advantage that y_{v_1} is directly related to a plant temperature measurement. Thus, Run 7 was established. Switching between steady state controls was performed in the same manner as for Run 6. Rather than start extreme action from a specific point in time, a specific value of $y_{v_1} = .675$ was chosen as an indication that new steady state control could not maintain the initial specification in face of the feed composition change. Runs were performed using $\phi = .65$ and various values of R_D from the final steady state value of .42869 to .65. $R_D = .55$ gave the best performance but values of $R_D = .50$ and $R_D = .60$ also yield reasonable results. This may be of importance from an implementation point of view since operators are naturally reluctant to use extreme action. Initially smaller values of R_D could be implemented but these could be increased as experience and confidence are gained.

The simulation of Run 7(d) is shown in Fig. 5.7. Comparison with the optimal responses in Fig. 5.4 illustrates that the general shape of the optimal curves have prevailed. From this sub-optimal run it is clear that conventional plant feedback control could be implemented from $t = 3$ hr.

Fig. 5.7 shows that maintenance of the initial kerosene and residue product specification during the top product changeover is somewhat erratic. Within the discussion of the optimal results it became apparent that the kerosene and light gas oil drawoffs could be utilized to control the set points of the kerosene and residue

Figure 5.7 Sub-optimal Concentration Responses For
Crude Change Subproblem (i) (Run 7d)



streams respectively. Runs 8 and 9 were performed under the same conditions as Run 7d) except proportional control was used on these two loops from time zero until the switch at $y_{v_1} = .45$. This led to OAF values up to .8492. Thus, an on-line algorithm is now established which utilizes conventional feedback control, plant temperature measurements, and feedforward control levels with switches governed by simple feedback laws.

5.4 Subproblem (ii) - Optimal Feed Flowrate Regulation Policies

The extremely fast responses in subproblem (i) were determined under the assumption that the feed flowrate change had already been undertaken. Subproblem (ii) is concerned with reaching the initial conditions of subproblem (i) from the initial conditions of the main problem; that is, maintain the specifications in face of a feed flowrate disturbance. Objective function and optimal control parameters are the same as those given in section 5.2.

The initial and final conditions for subproblem (ii) are shown in Table 5.5 and the inconsistency of specifications of crudes A and A₁ has already been discussed in section 5.3. Optimal control results are presented in Fig. 5.8-5.10.

The optimal objective function value is 1.176×10^{-4} compared with 4.991×10^{-4} for the application of steady state control. Steady state is restored within 0.5 hr. of the occurrence of the upset. It is worth noting that even the steady state control objective function value represents only 5.5% of the optimal objective function for the previous subproblem. This suggests that application of steady state control for this phase of the changeover would contribute little off-specification product within the context of the entire crude changeover period. If this policy is adopted,

TABLE 5.5 STEADY STATE CONDITIONS FOR CRUDE CHANGEOVER

SUBPROBLEM (ii)

Crude	A	A ₁
F (tonnes/hr)	470	360
z_{F1}	.170	.170
z_{F2}	.100	.100
z_{F3}	.100	.100
z_{F4}	.240	.240
z_{F5}	.390	.390
R (tonnes/hr)	109.00	70.00
R_D	.44103	.48905
R_N	.11788	.12306
R_{KERO}	.14697	.11807
R_{LGO}	.39646	.46502
D (tonnes/hr)	86.0	67.0
S ₂ (tonnes/hr)	15.0	10.0
S ₄ (tonnes/hr)	30.0	18.0
S ₆ (tonnes/hr)	100.0	96.0
B (tonnes/hr)	239.0	169.0
Q ₃ (thermies/hr)	9103.70	8000.0
Q ₆ (thermies/hr)	10400.00	9000.0
Q ₉ (thermies/hr)	-1444.47	-1444.47
ϕ	.52	.52
y_{v1}	.7435	.7321
x_{22}^*	.4594	.4485
x_{43}^*	.3522	.3433
x_{64}^*	.3770	.3691
x_{95}^*	.6809	.7012

 z_F - feed concentration R_D - distillate ratio R_N - drawoff ratio for S₂ R_{KERO} - drawoff ratio for S₄ R_{LGO} - drawoff ratio for S₆ ϕ - feed vaporization ratio

Figure 5.8 Optimal Concentration Responses For
Crude Change Subproblem (ii)

Upsets: $F : 470 \text{ t./hr.} \rightarrow 360 \text{ t./hr.}$ at $t = .5 \text{ hr.}$

$$I_{ss} = 4.991 \times 10^{-4}$$

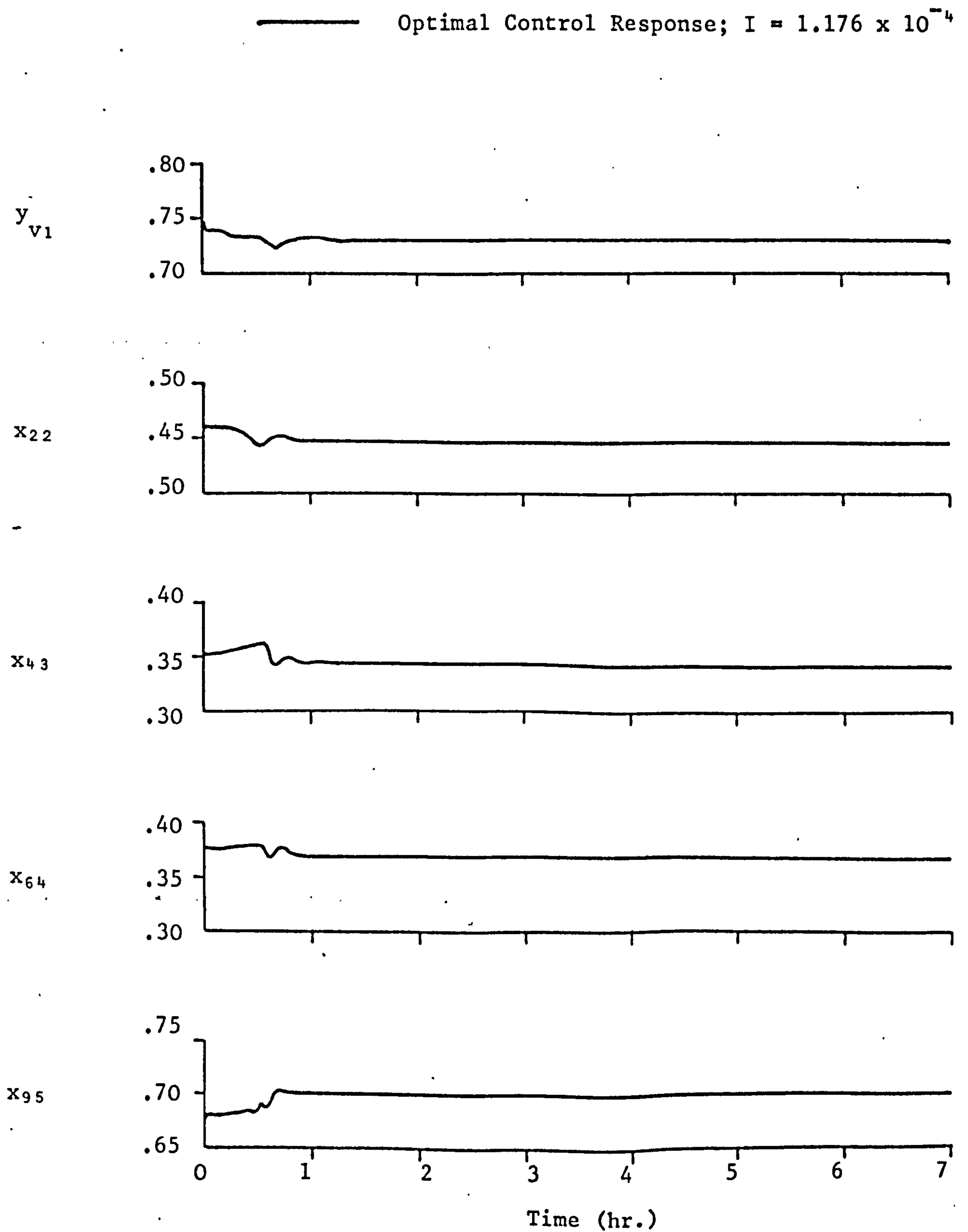


Figure 5.9 Optimal Flowrate Controls For
Crude Change Subproblem (ii)

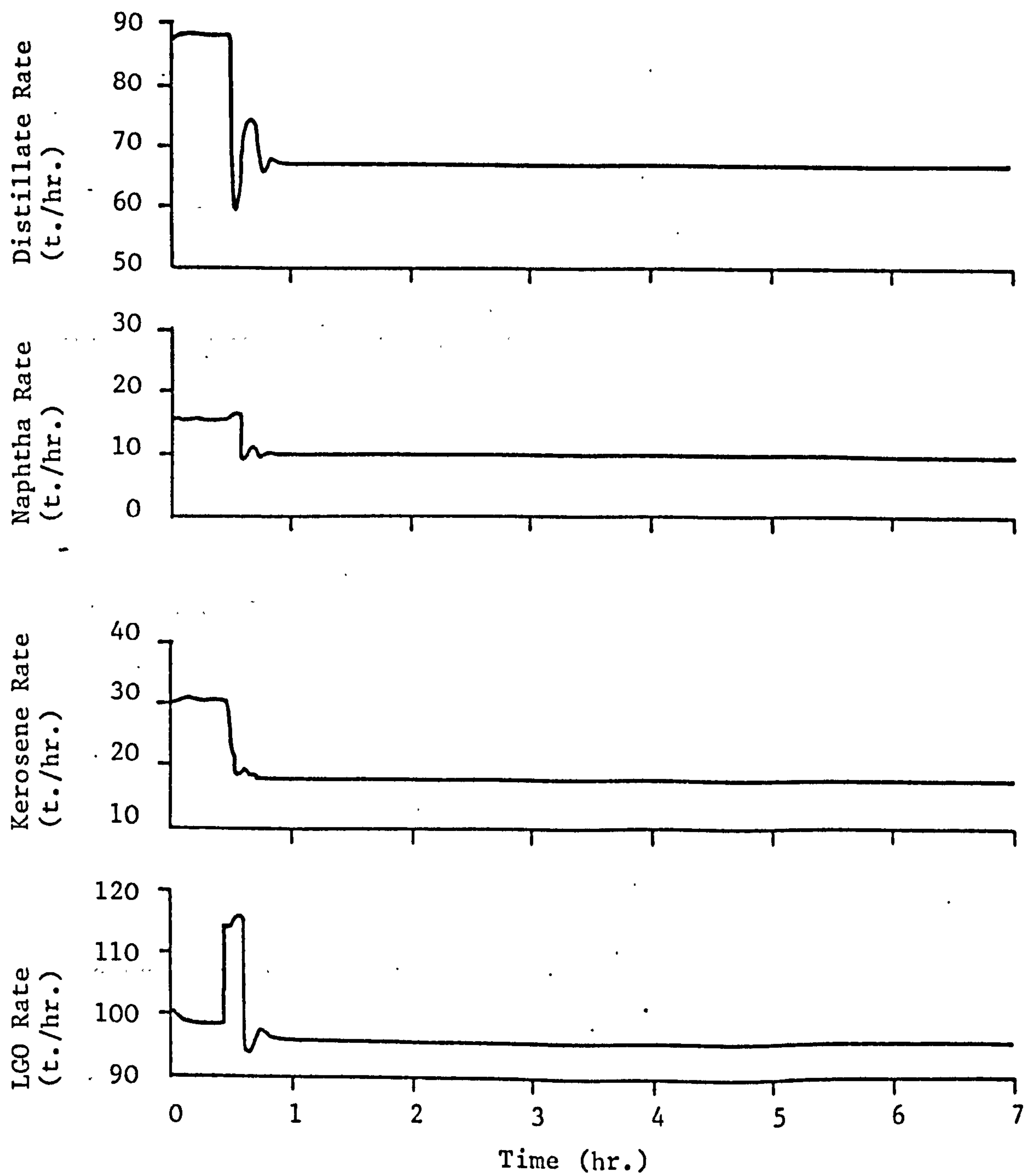
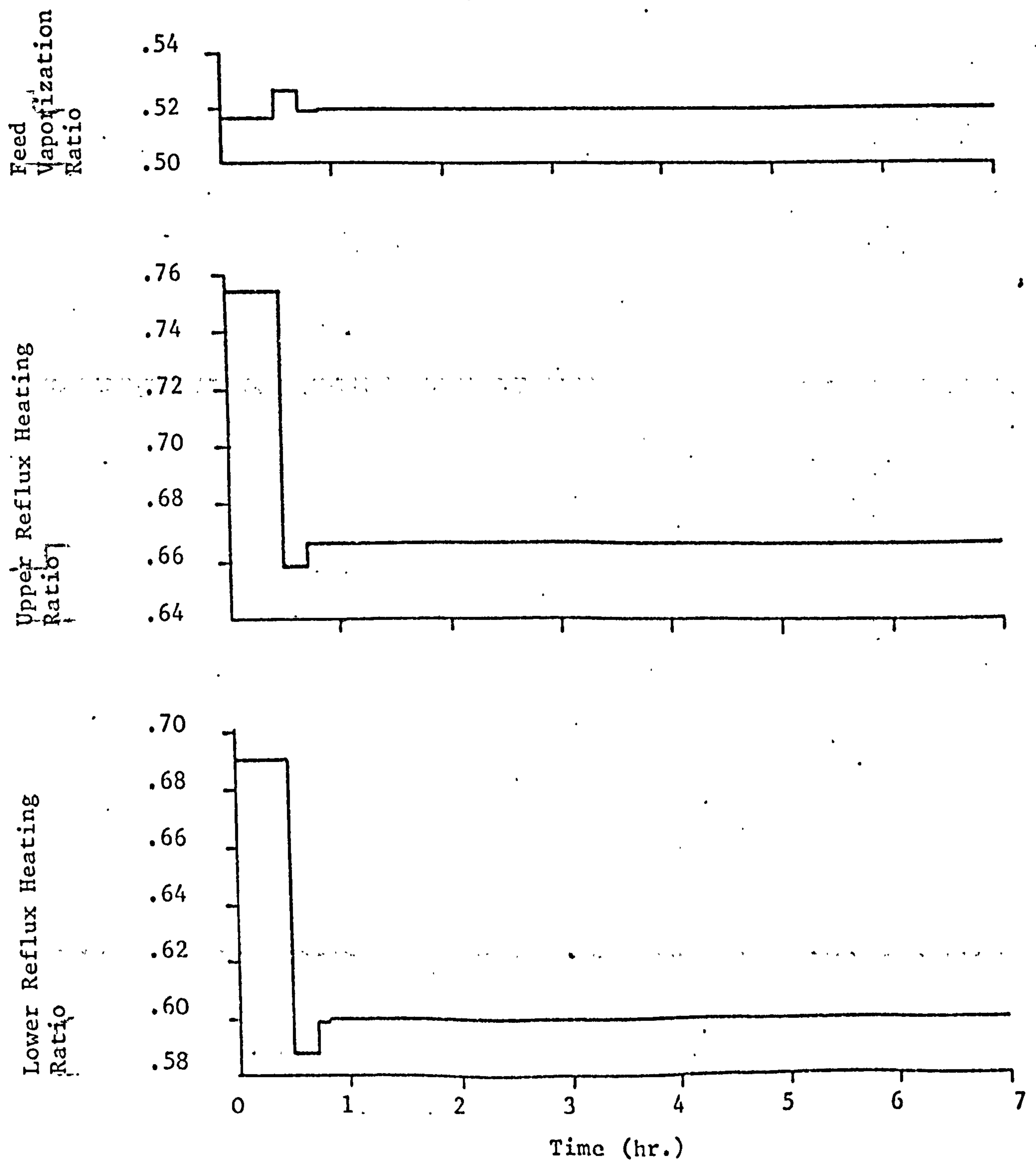


Figure 5.10 Optimal Heating Controls For
Crude Change Subproblem (ii)



it would be worthwhile to examine the influence of the steady state control switching time on the response performance.

Results in Table 5.6 show objective function values for various steady state control switching times. A minimum objective function value occurs at $t = 0.45$ hr., and this has a OAF value of .823. These results in Table 5.6 are based on the control ratios being switched between steady state values. Because of this, there is a short time lag before the drawoff rates reach the new steady state as is evident from Fig. 5.9. It is of practical interest to investigate the case where product flowrates are placed on new steady state at switch time. Objective function values for various switching times are also given in Table 5.6. Although a minimum occurs at $t = 0.5$ hours, the most striking feature is that all objective function values for the direct control case are approximately an order of magnitude higher than those for the ratio control case. There are some sound physical reasons for these observations. From the debutanizer study, it was shown that the optimal regulator for a load change was to lag the controls between the two steady states because the effect of the disturbance is lagged at the control location. Such a lag is inherent in ratio control: at a constant ratio, the product drawoff is altered with the internal liquid flow (or overheads vapour for the distillate).

There are many literature references on ratio control (Rademaker et. al. (1975) provide a good review), but these usually imply a ratio to the feed rate. A common exception is reflux ratio control. The results indicate that it is the close proximity of the reference variable to the control location which provides the

TABLE 5.6 OBJECTIVE FUNCTION VALUES FOR VARIOUS STEADY
STATE CONTROL POLICIES FOR SUBPROBLEM (ii)

Nature of Control	Switch Time (hr)	I
Ratio	.425	2.443×10^{-4}
	.450	1.794×10^{-4}
	.475	2.483×10^{-4}
	.500	4.991×10^{-4}
Direct	.450	2.547×10^{-3}
	.500	9.113×10^{-4}
	.550	2.456×10^{-3}

benefit from ratio control. From a practical viewpoint, it may be argued that internal liquid flowrates are difficult to measure. However, current control practice on the main column includes withdrawal from the the column, measurement, and return of the internal liquid flowrate (L_8). With measurements of L_8 and the reflux rate it may be possible to estimate the internal liquid flowrate profile. Under normal circumstances, maintenance of specification in the face of a feed rate change would involve no change in the drawoff control ratios (this was not the case here because of the constraint on Q_9). Hence, no control action need be applied; the drawoffs would change as the internal liquid flowrate changed.

The overall strategy for the crude change problem is now complete.

- (i) 0.5 hours before the crude changeover is scheduled to occur, change the feed flowrate of crude A to match the nominal feed flowrate of crude B. Change to interim steady state control a few minutes before the switch.
- (ii) Changeover to crude B and control according to policy outlined in section 5.3.1.

It is interesting to note that the overall optimal objective function from the addition of subproblems (i) and (ii) is 9.46×10^{-3} compared with 1.14×10^{-2} for the main problem. This illustrates the control benefit gained from separation of feed flowrate and feed composition changes. Addition of sub-optimal policies from Run 8c) in Table 5.4 for the composition change with a switch between steady state control ratios at the upset time for the feed flowrate change yields an objective function of 1.31×10^{-2} .

CHAPTER 6 - SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

The development of feed changeover policies for refinery distillation units has been undertaken. An efficient optimal control package was created and this was utilized to generate optimal open-loop responses for three distillation units under various conditions. Feedforward/feedback strategies were then devised which extracted the dominant features of the optimal responses yet allowed for the practical aspects of implementation.

The general conclusions and recommendations on the optimal control aspects of this work are as follows:

- 1) Optimal control problems with bounded controls, final time constraints, and path constraints can be formulated as a non-linear program using piecewise constant control levels and variable switching times. The novel formulation of path constraints as a final time constraint involved the addition of only one new state variable.
- 2) Linear multistep integration methods were examined in order to cope with stiff systems of differential equations which characterize many chemical engineering multi-stage operations. It was found that significant computational savings could be realized by utilizing working matrices on the reverse adjoint integration that were generated and used on the forward state integration. In fact, these savings were found not to be restricted to stiff systems, and up to ten fold reduction in computer time was exhibited by linear multistep methods over a fourth-order Runge-Kutta procedure on a non-stiff system. Optimal control procedures which update the control

vector using gradients are already accepted as the best available method. The integration algorithm developed in this work could act as a module within the framework of any of these procedures to yield even greater computational efficiency.

- 3) An algorithm has been presented to solve optimal control problems. Its efficiency has been demonstrated by application to a standard test problem and many distillation examples. The capability of the algorithm to deal with large multivariable systems is evident from the fact that the dynamic optimization of the main crude column represents the largest optimal control problem solved to date in the chemical engineering field. Since this work does not involve final time or path constraints the current version of OPCON does not allow for their existence. These could be included with relatively little coding effort, and the efficiency of the algorithm to solve problems with such constraints could subsequently be tested.

General conclusions and recommendations on the distillation control aspects of this work are as follows:

- 1) For profit type objective functions, a method has been developed that assigns marginal values and base values to product streams in order to ensure consistency between optimal steady states of linear program models used for overall plant optimization and dynamic models used for control purposes. This method could be used in any application that requires steady state optimality agreement between models which have been developed separately.
- 2) An optimal stream fractioning policy was developed for profit type objective functions and for the case where product values are related to component concentration via marginal values,

simple a priori product storage policies were derived. For deviation from set point type objective functions the same analysis results in a set point switching rule for changeover problems. This eliminates the need for a priori set point trajectories and allows more control flexibility in order to create faster changeovers.

3) Optimal control calculations performed on the three columns revealed the following results:

a) Advance information concerning the upsets and new steady state control settings is extremely valuable.

b) Regulator problems, where product specifications are to be maintained in the face of feed upsets, are best solved by moving controls between initial and final steady states via a first order lag. The time constant for the lag is dependent on the nature of the upset and size of the column.

When the number of control variables is greater than or equal to the number of state variables appearing in the objective function and the controls have a direct influence on these state variables (e.g. debutanizer), then all the control action can take place after the disturbance in order to cancel the effect of the upset. However, when the reverse situation occurs (e.g. splitter), control action prior to the upset time can be beneficial.

c) Fast changeover responses are effected by causing the entire contents of a column to become light together or heavy together. For cases where product streams are to become either all lighter or all heavier, extreme control action may be used to facilitate the changeover. When the specifications of product streams are not all to move in the same direction,

the set point switches are ordered so that the column contents still move light together and heavy together.

- 4) Implementable sub-optimal policies were developed for the debutanizer and main column in the form of feedforward control levels with switching between these levels governed by simple feedback laws. For the binary column, in which product streams were to become both lighter or both heavier, termination of extreme control action was signalled by the overshoot equals undershoot condition. This easily implementable law can be extended to multi-product columns by using a weighted sum of overshoots equals weighted sum of undershoots condition.
- 5) A strategy has been derived for control of an atmospheric crude oil distillation column subject to a changeover between dramatically different operating conditions. This strategy takes the form of maintenance of initial product specification, while feed flowrate changes are overcome, followed by product specification changeover in the face of feed composition changes. It would be of practical interest to perform the optimal control of the reverse changeover that was used as a basis for this work. However, the general trends and the control philosophies that have been discussed are likely to remain unaltered.
- 6) For the regulation of multi-product distillation columns in the face of feed flowrate upsets, control of the ratio of sidestream drawoffs to the internal liquid flowrate has been found to yield far superior performance to control of the sidestream drawoff rates directly. If the internal liquid flowrate could be estimated, then this benefit comes with no expense

for increased measurement effort.

Several logical extensions of this work are apparent. The optimal control package, OPCON, was developed for a fixed step size integration method whereas efficient procedures (e.g. Gear's method) could be utilized that rely on variable step sizes. This would serve several purposes. Firstly, parameters such as the frequency of relaxation matrix updates could be adjusted automatically with step size since changing step sizes reflect changing magnitudes within the Jacobian matrix. Also, since the step size is determined in order to integrate within a certain error tolerance, a variable error tolerance policy could be established. In this manner, inaccurate and inexpensive integration could be performed initially, with subsequent reduction of the error tolerance as convergence proceeds.

Work on implementation of the proposed strategy for the main column crude changeover has already been started on site by BP. It would be interesting to test the simple control laws that were developed for the debutanizer. However, some of the features concerning distillation extend beyond the three columns studied in this work. Such concepts as drawoff ratio control for multi-product columns, moving contents of columns lighter and heavier together to effect faster responses, and the undershoot equals overshoot conditions, apply to distillation in general. Independent work, perhaps on pilot plant columns, to validate these findings would be beneficial.

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