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A MULTICOMPONENT DISTILLATION COLUMN SIMULATOR FOR STUDIES IN DYNAMICS AND CONTROL

by

GLYNIS A. CARLING

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A THESIS
SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH
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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled A MULTICOMPONENT DISTILLATION COLUMN SIMULATOR FOR STUDIES IN DYNAMICS AND CONTROL submitted by GLYNIS A. CARLING in partial fulfilment of the requirements for the degree of MASTER OF SCIENCE in PROCESS CONTROL.

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Supervisor

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Date 26 September, 1986

Abstract

A simulator, known as DYCONDIST, has been developed at the University of Alberta to model dynamic behaviour of multicomponent distillation columns. In this work enhancements made to the simulator to facilitate investigation of column dynamics and control are described as are results obtained by applying the package to open and closed loop studies of a 31 stage depropanizer.

Open loop study of the tower consisted of simulation of dynamic responses to feed rate disturbances as well as to step changes in reflux rate and reboiler duty. The base case column feed consisted of five components, but the sensitivity to the number and distribution of feed species was also considered for a feed rate decrease. In some of these cases inverse composition responses are exhibited and, although this behaviour was mainly restricted to the key components in the column sections they dominate, inverse responses of non-key components and even of stage temperatures were observed for some five component feed disturbance cases. The inverse behaviour was predicted regardless of whether constant or variable stage liquid holdup was assumed. Some generalizations are made about the effects of disturbance type and size and feed characterization on the prediction of nonminimum phase behaviour.

Control schemes implemented as part of the closed loop study of the depropanizer ranged from conventional to

advanced strategies including local level control, single and dual quality control and feedforward compensation as well as a self-tuning control algorithm. Although optimal controller tuning was not performed, some improvement was seen when using direct composition measurements as opposed to temperature feedback control. Relative gains and relative disturbance gains were calculated for the dual quality control cases, but little correlation was found between these measures and simulation results. Feedforward control provided considerable improvement in performance over feedback control alone. Performance of the self-tuning controller was comparable to that of the conventional schemes, but it is felt that this could be improved by optimal design of the weighting parameters used in the algorithm.

The simulator has been demonstrated to be very useful in distillation column control system design as well as in the development and testing of advanced control techniques. Some suggestions are given for future work.

Acknowledgements

The financial support of the Department of Chemical Engineering during the course of this work is gratefully acknowledged. Many thanks are also due to Dr. R. K. Wood for his time, effort and guidance as my supervisor. The support and encouragement of family and friends has been greatly appreciated and the opportunity to learn from and exchange ideas with various professors and fellow students has made the past two years a tremendous experience.

Special thanks to the eighth floor crew and to Dave, Dave and Bill who helped keep everything in perspective.

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Nomenclature and Notation

a	coefficient used in ASIRK integration as defined for use in Equations (2.15) and (2.16)
a_0, a_1	coefficients in the polynomial used for component liquid enthalpy correlation (Equation 3.1)
a_{ij}	interaction coefficient for components i and j used in Wilson equation (Equation 2.14) to calculate the activity coefficient for component i
$A(z^{-1})$	polynomial matrix used in self-tuning control model equation (4.14)
b	coefficient used in ASIRK integration as defined for use in Equation (2.16)
b_0, b_1, b_2	coefficients in the polynomial used for component vapour enthalpy correlation (Equation 3.2)
B	bottoms product rate
$B(z^{-1})$	polynomial matrix used in self-tuning control model equation (4.14)
BIAS	steady state control action

BTM IAE	integral of the absolute deviation between the impurity mole fraction in the bottoms product and the desired impurity specification
c_0, c_1, c_2	coefficients in the polynomial used for component equilibrium ratio correlation (Equation 3.3)
c_k	controlled variable for control loop k. (This will be a temperature for indirect control and a component mole fraction for direct control).
$C(z^{-1})$	polynomial matrix used in self-tuning control model equation (4.14)
Cp_j	heat capacity of liquid on stage j
CONTR	controlled variable
D	liquid distillate rate
$D(z^{-1})$	polynomial matrix used in self-tuning control model equation (4.14)
e_j	truncation error estimate for the j^{th} equation in a set of equations integrated using ASIRK integration
$\mathbf{e}$	vector of truncation error estimates for the set of differential equations integrated using ASIRK integration
E_j	coefficient in energy balance equation (2.4) for stage j

ER	control error (difference between the setpoint and feedback signal)
f	vector of functional values for ASIRK integration
F	feed flow rate
F_j	feed flow rate to stage j
$\hat{F}(z^{-1})$	estimated matrix of model parameters for self-tuning control law equation (4.15)
G_{ij}	function of interaction coefficient, a_{ij}, and molar volumes of components i and j used in Wilson equation to calculated the activity coefficient for component i
$\hat{G}(z^{-1})$	estimated matrix of model parameters for self-tuning control law equation (4.15)
h	time step for ASIRK integration
h_j	liquid enthalpy on and leaving stage j
h_{fj}	liquid enthalpy for feed entering at stage j
H_j	vapour enthalpy leaving stage j
$\hat{H}(z^{-1})$	estimated matrix of model parameters for self-tuning control law equation (4.15)
HK	heavy key component
I	identity matrix
J	Jacobian matrix for ASIRK integration
k_1, k_2	increment functions for ASIRK integration
K_d	PID controller derivative action constant
K_i	PID controller integral action constant
K_i	equilibrium ratio for component i

K_p	PID controller gain
K_{ij}	steady state gain between the ith controlled variable and the jth manipulated variable where j=1,2 for control loops 1 and 2 and j=3 for the disturbance variable, feed rate
L_j	liquid rate leaving stage j
L_B	column base surge level
L_C	condenser level (flooded condenser)
L_D	accumulator level
$\hat{L}(z^{-1})$	estimated matrix of model parameters for self-tuning control law equation (4.15)
LK	light key component
LOOP IAE	integral of absolute deviation of controlled variable from its setpoint for a given loop
m_k	manipulated variable for control loop k
M_j	liquid molar holdup on stage j
MANIP	manipulated variable
N	total number of stages in a column
NC	total number of components in a multicomponent mixture
OP	controller output
P	column pressure
$P(z^{-1})$	polynomial matrix used in self-tuning control law to provide weighting on system outputs
P_d	denominator of $P(z^{-1})$ polynomials used in self-tuning control
Q	product quality

Q_B	bottom product quality
Q_D	liquid distillate product quality
Q_j	heat loss from stage j
$Q(z^{-1})$	polynomial matrix used in self-tuning control law to provide weighting on control action
QR	reboiler duty
R	reflux rate
$R(z^{-1})$	polynomial matrix used in self-tuning control law to provide weighting on setpoints
s_j	liquid sidedraw rate from stage j
S_j	vapour sidedraw rate from stage j
SP	setpoint
t	time
T_j	liquid temperature on stage j
TEMP	stage liquid temperature
TOP IAE	integral of the absolute deviation between the impurity mole fraction in the liquid distillate product and the desired impurity specification
U(t)	vector of control actions for self tuning control
V_D	vapour distillate rate
V_j	vapour rate leaving stage j
V(t)	vector of measurable disturbances for self-tuning control
w	coefficient used in ASIRK integration as defined for use in Equation (2.17)

w_1, w_2	coefficients for ASIRK integration as defined for use in Equation (2.19)
$W(t)$	vector of setpoints for self tuning control
x_j	a single component mole fraction for liquid on and leaving stage j
$\underline{x}_j$	vector containing mole fraction of each component for the liquid on and leaving stage j
y	vector of solutions to a set of differential equations for ASIRK integration
y_j	solution to the j^{th} differential equation for ASIRK integration
y_j	a single component mole fraction for vapour leaving stage j
$\underline{y}_j$	vector containing mole fraction of each component for the vapour leaving stage j
$Y(t)$	vector of process outputs for self-tuning control
$Y^*(t)$	desired process outputs for self-tuning control
z	liquid level
z_j	a single component mole fraction for feed to stage j
$\underline{z}_j$	vector containing mole fraction of each component for the feed to stage j
$z^{-d_{ij}}$	system delay between the i^{th} measurable disturbance and the j^{th} process output

$z^{-k_{ij}}$	system delay between the i^{th} manipulated variable and the j^{th} system output

Subscripts:

i	denotes component number
ij	pertains to interaction between the i^{th} and j^{th} species in a multicomponent mixture
j	denotes a stage number OR the j^{th} equation in a set
s	pertains to the stiffest differential equation in a set

Superscripts:

n	denotes time increment for the integration of differential equation(s)
SP	denotes the setpoint for the superscripted variable
t	denotes the transpose of the indicated vector

Greek Letters:

α_j	coefficient in energy balance equation (2.4) for stage j
β_j	coefficient in energy balance equation (2.4) for stage j
β_1, β_2	relative disturbance gain for loops 1 and 2 as defined by Equations (5.2) and (5.3)
γ_i	activity coefficient for component i

γ_∞	limiting characteristic value for ASIRK integration
Γ_{ji}	intermediate term corresponding to stage j and component i as defined by Equation (2.13) and used in calculation of energy balance equation coefficients
λ_s	pseudo-eigenvalue of the stiffest equation in the set for ASIRK integration
λ	relative gain as defined by Equation (5.1)
Λ	relative gain array
ν_j	molar volume of component j
ξ_j^k	intermediate terms defined by Equations (2.9) to (2.12) for k=1,4 and used in calculation of energy balance equation coefficients
$\Xi(t)$	vector of random noise inputs for self-tuning control
σ	step size control parameter for ASIRK integration
ψ_j	coefficient in energy balance equation (2.4)

1. INTRODUCTION AND LITERATURE REVIEW

Distillation has long been the subject of academic and industrial research for two reasons: the process plays a key role in many chemical and petrochemical industries; and it is an energy intensive operation. Confronted with rising fuel costs, refiners and chemical processors have been motivated to determine efficient operating strategies. Knowledge of dynamic column behaviour is an important aspect of the development of improved distillation control schemes.

This work continues the development of a dynamic multicomponent distillation column simulator at the University of Alberta. Original development of the simulator, known as DYCONDIST, was performed by Wong (1985) and in this work modifications have been made to facilitate dynamic and control studies needed to keep pace with demand for efficient distillation column control strategies.

The background against which this work was undertaken is outlined in Section 1.1 and 1.2 in which contributions to the study of distillation column dynamics and distillation column control are discussed. These sections highlight the fact that a general purpose simulator such as the one used in this work is not currently readily available and does have the potential of being extremely useful.

A discussion of the assumptions on which the simulator is based is given in Chapter 2 along with an outline of the numerical methods and overall solution procedure used. This chapter also contains an outline of modifications and enhancements made to the DYCONDIST package during the course of this work.

Use of the simulator for dynamic studies is illustrated by example in Chapter 3. The column studied is a depropanizer about which details have been previously published (Ballard *et al.*, 1978; Cook, 1980; Wong and Wood, 1985). Because the column displays unusual dynamic behaviour in response to some disturbances, Chapter 3 also outlines an investigation into the inverse composition and temperature responses which were observed. The investigation is by no means exhaustive but does involve study of the effects of the number and distribution of feed components on the nonminimum phase behaviour observed.

The final two chapters of the thesis are devoted to use of the simulator for control studies. Chapter 4 outlines modifications made to DYCONDIST to implement a variety of local and remote control algorithms. An example is included in which the material balance equations are tailored to incorporate local level control at the overhead accumulator.

The depropanizer column used in the dynamic behaviour study is again used in Chapter 5 to illustrate the use of the simulator for control studies. The control strategies considered start with basic material balance or inventory control and progress to single product quality control and to dual product quality control. Interaction analysis using steady state operability measures is also discussed. Finally, DYCONDIST is used to simulate feedforward and self-tuning control strategies applied to the depropanizer as examples of the study of advanced control techniques.

1.1 Dynamics of Multicomponent Distillation

1.1.1 Overview

Work in the field of distillation research has progressed parallel to advances in computing technology. Before the advent of fast, relatively inexpensive digital computers, attention centred on simplified approaches, usually dealing with binary or pseudo-binary distillation. Because of the complexity of rigorous calculations, methods of interest involved shortcut steady state calculations.

Holland (1983) notes that the theory of distillation was first studied by Sorel in 1893. Early design techniques were based on the work of Lewis and Lord Rayleigh. Graphical techniques were developed by Ponchon and Savarit and by McCabe and Thiele in the 1920's for binary separations. Work on multicomponent distillation generally involved approximate models or empirical methods such as that developed by Smith and Brinkley, or the combination of Fenske's total reflux equation, Underwood's minimum reflux equation and the Erbar-Maddox graphical method (Smith, 1973).

Work on dynamic multicomponent distillation simulation dates to the 1960's. Rosenbrock (1962) outlined three possible methods for the investigation of column transient behaviour: calculation of frequency response; use of a passive analog; or direct solution of the governing equations. He concluded that none of the methods was quick or cheap enough for routine use. He recommended that approximate models be used to represent the primary and secondary aspects of column behaviour. This avoided direct calculation of transient behaviour until an efficient computation procedure could be developed.

In contrast, Peiser and Grover (1962) were prompted by control problems with an operating tower to study the tower dynamics. They approached the problem by solving the equations describing both the tower and auxiliary equipment. As a result of their open and closed loop studies they were able to redesign the tower trays, eliminating the control problems.

Tetlow *et al.* (1967) developed a generalized computer model for simulation of dynamic column behaviour. Their model was complex, taking into account mixing effects on the plates as well as in downcomer, reflux drum and transfer line holdups. Mixing effects were described as a linear combination of three limiting cases: perfect mixing; plug flow; and channeling.

Howard (1970a) summarized contributions to the field to that date. He presented a generalized model incorporating three different liquid holdup models. His attempt to match predicted behaviour with that observed experimentally met with limited success (Howard, 1970b). Differences were attributed to the use in the computer model of inadequate information about the experimental column.

The value of rigorous dynamic multicomponent distillation modelling is now generally recognized. The benefits obtained are a further understanding of column operation and a basis for the establishment of column control strategies. Various studies of particular columns have been reported over the past decade. Ballard *et al*. (1978) simulated a depropanizer as part of their work developing an efficient simulation algorithm. Gallun (1979) simulated closed loop performance of an extractive distillation column separating acetone from methanol and ethanol using water as the extractive agent. This work is also described in detail by Holland and Liapis (1983) and Wong (1985) duplicated their results with the simulator used in this work. Prokopakis and Seider (1983) developed a simulator for an azeotropic distillation tower and Kumar *et al*. (1984) reported on experimental and simulation studies of an extractive column. Stathaki *et al*. (1982, 1985) simulated the dynamic behaviour of an industrial column, finding that asymmetric dynamics were a distinguishing feature of the system they studied. Ralston (1983) studied an industrial de-ethanizer and used the results to modify the column's control strategy (Ralston *et al*., 1985).

As indicated, each of these simulation programs has been developed to study a specific column. A general purpose dynamic simulator which could be easily applied to the study of a wide variety of columns would be ideal. The development effort required for such a general purpose simulator has been justified by a number of corporations and proprietary simulators have been applied to a variety of problems (Moser, 1982; Cheung and Marlin, 1982; Wei, 1985). The fact that these packages are not generally available led to the initiation in 1983 of work at the University of Alberta on the development of a general purpose dynamic simulator for multicomponent distillation. This simulator has been applied to the study of a number of columns including an extractive distillation column, a two column industrial unit, and a pilot scale water-methanol column (Wong, 1985), as well as the depropanizer discussed in this work (Wong, 1985; Wong and Wood, 1985).

The dynamic simulation studies cited above have involved a variety of assumptions and numerical methods. A discussion of the selection of an appropriate set of assumptions on which to base a dynamic simulation is presented in Section 1.1.2. Some insight into the use of rigorous as opposed to reduced models is given in Section 1.1.3. The selection of numerical methods used for rigorous column simulation is discussed in Section 1.1.4. Finally, nonminimum phase behaviour relating to distillation studies is discussed in Section 1.1.5.

1.1.2 Assumptions

The assumptions required for rigorous digital computation of multicomponent unsteady state distillation are much less restrictive than were those required to obtain solutions in a reasonable time frame using computing facilities less advanced than those available today. Shortcut approaches include assumptions of constant molar overflow for all trays or for trays in a given column section, representation of the feed mixture as pseudo-binary, and assumptions of constant liquid enthalpy and/or holdup. As discussed in Section 1.1.3, some of these approaches are used in reduced order distillation models.

Today's computer resources make rigorous calculations feasible. However a trade-off must still be made so that results of the desired degree of accuracy are obtained as quickly and cheaply as possible.

Any simplifying assumption made to speed computation will have some effect on the results. The importance of the effects of most of the common assumptions have been addressed by various researchers. The assumptions made by selected workers, as summarized in Table 1.1, will now be discussed.

- MIXING EFFECTS

  It is generally assumed that the liquid on a stage is well mixed since it is continuously agitated by vapour passing through it. Tetlow *et al.* (1967) investigated

Table 1.1

DYNAMIC MULTICOMPONENT DISTILLATION MODELLING ASSUMPTIONS

SIMPLIFYING ASSUMPTIONS:	Peiser and Grover (1962)	Waggoner and Holland (1965)	Tetlow et al. (1967)	Howard (1970a)	Ballard et al. (1978)	Gallun (1979)	Morris and Svrcek (1981)	Ralston (1983)	Holland and Liapis (1983)	Wong and Wood (1985)	Stathaki et al. (1985)
Perfect mixing	Y	Y	N	Y	Y	Y	N[1]	Y	Y	Y	Y
Negligible vapour phase material and energy holdup	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
All stages ideal (100 tray efficiency)	P	N	N	N	Y	Y	N	Y	Y	P	Y
Negligible thermal capacity of tower internals	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Negligible tray heat loss	Y	Y	Y	N	N	Y	N	Y	Y	P	Y
For tray liquid holdup:											
1. Constant molar holdup	N	P	N	P[2]	P	P	N	N	P	P	N
2. Constant volumetric holdup	N	P	N	N	N	N	N	N	P	N	N
3. Constant mass holdup	N	P	N	N	N	N	N	N	P	N	N
4. Holdup related to liquid rate	N	N	P	N	N	N	N	N	N	N	Y
5. Holdup from Francis weir equation	Y	N	Y	N	P	Y	Y	Y	P	P	P
No volume change on mixing	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Constant linear pressure drop	U	U	Y	Y	U	P	N	Y	P	P	Y

Legend:

Y	assumption incorporated
N	assumption not incorporated
P	assumption optional
U	assumption unknown

Notes:

1. Perfectly mixed layers of liquid assumed.
2. Holdup was alternatively described by as varying exponentially with time.

mixing effects, but later work by Holland and co-workers abandoned this approach (Holland and Liapis, 1983). Morris and Svrcek (1981) assumed that the liquid on each tray was composed of layers of varying thicknesses. This was in order to use their semi-empirical non-equilibrium vapour-liquid relationship rather than to avoid making the perfect mixing assumption.

- VAPOUR HOLDUP

Since any vapour holdup on trays is much smaller than the liquid holdup, it may be assumed that the effect of vapour holdup is negligible.

- TRAY EFFICIENCY

While many workers incorporate a Murphree efficiency option in their column models, it appears just as common to account for the nonideality of real stages by using an assumed efficiency factor to represent the ratio of the number of simulated stages to the actual number of stages. (i. e. the real tower stages are represented by the appropriate number of ideal stages). The efficiency factor may be based on experimental observation of the tower performance, or may be an estimate based on the type of tower in question. Other approaches used have been to correlate efficiency to the composition of a specific stage (Wong, 1985), or to use a semi-empirical model to simulate the non-equilibrium stages (Morris and Svrcek, 1981).

- THERMAL CAPACITY OF TOWER INTERNALS

Most researchers have neglected energy holdup in tray and downcomer metal for multicomponent distillation work. Rademaker *et al.* (1975) included the heat capacity of tray metal in their development of the energy balance equation accounting for small differences in the pressure and temperature of the two phases on a tray. This nonequilibrium behaviour is assumed to affect only temperatures and pressures because of the slower dynamics involved for composition changes. The principal time constant they derived for these deviations has a value of about half a second in their example. Simonsmeier (1978) investigated the effect of energy storage in tray metal for binary distillation and found it to be negligible.

- LIQUID HOLDUP CORRELATIONS

Although some workers have considered using constant mass or volumetric liquid holdup specifications (e. g. Waggoner and Holland, 1965), constant molar holdup appears to be the most commonly accepted constant holdup assumption used. Results of this work include a study of the effect of constant versus variable molar holdup.

Where variable liquid holdup is assumed, some form of the Francis weir equation is generally used to correlate liquid holdup to flow rates. As an exception, Howard (1970a) considered liquid holdup as an exponential function of time. Other options such as the AIChE bubble cap tray design formula have also been used (Simonsmeier, 1978).

- PRESSURE DROP

  Rather than a rigorous calculation of column pressure variation with time, it is commonly assumed that column pressure profiles are linear and constant. This is equivalent to assuming ideal pressure control at all times.

1.1.3 Reduced Models

It is instructive to consider the derivation and use of reduced distillation models for two reasons. First, a large effort is involved in rigorous calculations and alternatives should be understood before making that effort. Second, one of the objectives of reliable rigorous models is that they may be used to develop and test reduced models. There is a need for these models independent of rigorous models since they may be used for on-line optimization and/or for adaptive control.

Various approaches have been used to develop low order distillation models. Moczek *et al.* (1963) reported on study of reduced models developed by fitting first, second and higher order models to response curves calculated using a rigorous model with constant liquid holdup. For cases in which first and second order models proved inadequate, higher order models were fit using an analog computer. The study resulted in reasonable models for disturbances in reboiler duty and feed composition and for step changes in distillate and sidedraw rates. The column studied was a benzene-toluene-xylene separation column. The model order, time constants and time delay varied with input type and with the direction of change in the input variable. For this reason the models would be inappropriate for optimization or control applications.

Duyfjes and van der Grinten (1973) worked on reduced binary distillation models for use in control applications. They based their models on shortcut calculation methods to include nonlinear effects. Extension of this work to multicomponent distillation would prove difficult since shortcut methods for multicomponent distillation are necessarily more complex than those for binary distillation.

Other approaches have been used more recently. Eitelberg (1981) studied model reduction techniques for high order linearized models. A forty-fifth order distillation model was used as an example. The method was based on the minimization of weighted equation error and could be useful for columns operating in a linear region.

A method described by Gilles and Retzbach (1983) used a full dynamic model of a extractive distillation column to yield steady state and transient temperature and composition profiles. These profiles were then used as the basis for division of the column into sections about which overall balances were written. Solution of these balances provided a reduced order model. The method is, however, restricted to columns with sharp temperature profiles.

Cho and Joseph (1983a) compared three methods of establishing reduced order models and applied them to nonlinear multicomponent columns (Cho and Joseph, 1983b). Two of these methods depend on consideration of a distillation tower as a distributed parameter system. Composition and flow profiles are assumed to be continuous functions of column height which permits either the description of column profiles as polynomials or the expression of column dynamics as partial differential equations. The third method discussed by Cho and Joseph is the orthogonal collocation method used by Wong and Luus (1980). A problem with this method was found in that steady state material balances were not always preserved. Of the two distributed parameter methods, direct evaluation of polynomial functions representing column profiles provided better results than did solution of partial differential equations. More recent work (Cho and Joseph, 1984) featured applications their preferred method to columns with multiple feeds and sidestreams.

Although not extensive, this review of reduced order modelling provides background helpful when considering the potential role of a rigorous dynamic simulator in overall control system design and implementation.

1.1.4 Numerical Methods

The derivation of unsteady state column models (as discussed in Chapter 2) results in a set of algebraic and ordinary differential equations. Solution of the ordinary differential equations is of particular interest because of the fact that there is often great variation in the eigenvalues of the equations. (i. e. the equations are stiff). Special numerical methods are required since the alternative is to use an excessively small integration interval.

A large number of papers have been published on the solution of stiff ordinary differential equations (e. g. Chan *et al.*, 1978). For distillation calculations there appear to be two different approaches, judging by recent publications. Some researchers have used linear multistep methods based on Gear's method (e. g. Gallun, 1979; Gallun and Holland, 1982; Downs and Vogel, 1985; Kumar *et al.*, 1984) whereas other workers have used one of the semi-implicit Runge-Kutta (SIRK) methods (e. g. Prokopakis *et al.*, 1980; Wong, 1985; Ballard *et al.*, 1978). Both methods have been seen to be promising for simulation of dynamic separation processes (Holland, 1983). Prokopakis and Seider (1981) found their adaptive semi-implicit Runge-Kutta (ASIRK) method competitive with, and in some cases more efficient than, the Gear code. Wong (1985) compared ASIRK with Holland's iterative θ-method of convergence and with a fixed parameter SIRK method. He concluded that the ASIRK method performed better than the other two methods for the example used. (The example was one previously used by Holland and Liapis, 1983).

A brief list of references for the multistep and semi-implicit Runge-Kutta methods will be given here since the superiority of one over the other can not be presumed for all cases.

Gear Method

The Gear method was described in a series of articles by Gear (1967, 1971a, 1971b). It permits simultaneous solution of algebraic and differential equations and is implicit. Holland (1983) presented the simple example of a component material balance for a perfect mixer with constant holdup at unsteady state operation. Application to distillation has been discussed by Gallun and Holland (1982) and Gallun (1979) used the method to model an extractive distillation column. Byrne *et al*. (1977) compared the performance of the Gear algorithm to that of another multistep predictor method, the EPISODE code.

Semi-Implicit Runge-Kutta Methods

Rosenbrock (1963) created implicit analogs of the explicit Runge-Kutta method which avoided iteration in the solution procedure. Later investigations of this approach led to third and fourth order SIRK methods but few which could be successfully used to deal with nonlinear problems (Caillaud and Padmanabhan, 1971; Cash, 1976). Modifications made by Michelsen (1976) included the addition of a variable step size which improved results for nonlinear problems. A review of numerical methods for stiff equations found that SIRK methods are intrinsically efficient and easy to implement (Chan *et al.*, 1978). Chan and co-workers did not compare the computing efficiency of these methods with Gear's method and other commercially available software because the latter have been fully optimized whereas the available SIRK code had not.

Prokopakis and Seider (1981) introduced the adaptive SIRK method used in this work. In this method the stiff variable (i. e. that having the greatest percentage change in the current time step) is tracked. Its eigenvalue, approximated by a "pseudo-eigenvalue", is used to update the parameters in the standard Runge-Kutta incremental functions. This procedure has been found to perform well on nonlinear systems (Prokopakis and Seider, 1981; Wong, 1985).

1.1.5 Nonminimum Phase Behaviour

Reports of nonminimum phase behaviour of distillation columns and/or asymmetric distillation dynamics have been published but are not extensive. An exception is the inverse response of column base surge level and low-boilers in reponse to boilup increases which has been well documented. However, inverse response of compositions and temperatures have also been noted as have cases of asymmetric dynamics. These reports will be discussed here as the presence of these phenomena is a factor in the design of control systems.

Inverse response of base surge level in response to increases in boilup was first reported by Rijnsdorp in 1958 (Rademaker *et al.*, 1975). The inverse response phenomenon discussed by Rademaker *et al.* (1975), Luyben (1973) and Buckley *et al.* (1975) is considered to occur due to the "K_2 effect". Internal reflux on a given stage is a function of both the vapour rate from the stage below and the liquid rate from the stage above. When boilup is increased, liquid rates at the column base can increase for a time as the vapour term dominates. (Luyben, 1973). This has not been the only explanation offered. Rademaker *et al.* (1975) cite a case where a similar phenomena could not be attributed to the K_2 effect as the inverse response was not observed if feed temperature were controlled. They concluded that the inverse response behaviour was due to interaction with bottom level control by reboiler heating since in this particular case the reboiler tubes were mounted in the column bottom. Shinskey (1984) explains the phenomenon by noting that froth density will decrease as boilup is increased. If froth height changes more than the pressure drop across the tray changes then froth will spill over, increasing internal reflux. He claims that this can occur with sieve trays operating at low vapour rates as well as with valve trays. Control schemes designed to overcome this type of inverse response have been suggested by Luyben (1969a), Buckley *et al.* (1975) and Shunta (1985).

Observations of inverse composition responses have been noted in the literature. Waller and Gustafsson (1972) observed nonminimum phase behaviour of compositions in response to feed flow rate changes for partially vapourized feeds. They found that nonminimum phase behaviour was predicted for any components except those which dominated and were considerably enriched in the column section considered. Their work was, however, based on a simplified simulation which neglected column energy balances. Constant flow rates were assumed in each column section (Waller and Gustafsson, 1971). On this basis, it was concluded that irregular behaviour may be predicted on stages:

- which are near an extremum in the steady state composition profile and where system gains are small.
- where system gains are small and change sign.

It is difficult to have confidence in extending these results due to the restrictive assumptions of the model on which they were based.

Prokopakis and Seider (1983) noted inverse response in compositions when simulating an azeotropic distillation subjected to a thirty percent feed rate increase. They attributed the observation to a "washout" phenomenon, assuming that light components were being swept down the column by increased feed liquid. These authors also comment on inverse response in the work of Peiser and Grover (1962). It is unclear whether they had access to data additional to those published by Peiser and Grover, but examination of the figures in the published work does not lead to conclusions about the presence or absence of nonminimum phase behaviour.

Recent work by Stathaki *et al.* (1985) included observation of inverse response behaviour and asymmetric dynamics. In the simulation of a 20-tray industrial column Stathaki (1982) found that key components exhibit inverse response in the product streams they dominate. In addition, the column's dynamic behaviour was found to be sensitive to the distribution of key components in the column. Slow dynamics were observed when a step change in reflux, feed or Dowtherm flow rate caused the column to move towards a point of maximum separation. "Maximum separation" is defined as that state with maximum mole fraction of the light key in the distillate and of the heavy key in the bottoms (Stathaki, 1982).

As discussed by Wong (1985) and in this work, inverse responses of compositions in product streams and on intermediate stages have been noted in simulation of a depropanizer example. In addition, inverse temperature responses have been observed. Experimental verification of these phenomena would be helpful, but is difficult to obtain since open loop dynamic testing is required to observe inverse responses.

1.2 Control of Multicomponent Distillation

Control of distillation columns has been of great concern ever since the process came into widespread use. As a result, it has been the subject of numerous articles and books. Contributions to the distillation control literature have come from both the industrial and academic perspectives and have included reports on co-operative studies. Since the literature is so diverse, it has been unusual to find reviews putting the entire field into perspective. Various papers (Buckley, 1983, 1978; Mollenkamp and Waggoner, 1972; Tolliver and McCune, 1978; Tolliver and Waggoner, 1980; McAvoy and Wang, 1986) and recent books (Buckley *et al.*, 1985; Deshpande, 1985; Shinskey, 1984; Nisenfeld and Seeman, 1981; Rademaker *et al.*, 1975) have discussed distillation control. They have outlined control strategies and objectives in a very thorough manner. Unfortunately, all use different nomenclature and it is difficult to make meaningful cross-references. A critical review would be helpful, but would be an enormous task. The most recently published review (McAvoy and Wang, 1986) outlines distillation literature contributions in the period 1980-1984 using the categories established by Tolliver and Waggoner (1980). The reviewers do not, however, attempt to present a framework within which the papers they cite should be judged.

The objective of this literature survey is not that it should form a comprehensive review, but that it should serve to establish the control nomenclature used in this work and provide a basis for the control strategy selection made in this work. A brief look at the background of distillation control and the factors influencing the current "state of the art" will be presented first, with discussions of "conventional" and "advanced" control techniques to follow.

1.2.1 History of Distillation Control

In order to see why distillation control has developed as it has, it is instructive to consider some of the factors motivating work in the subject area. These can be grouped into three categories:

- Increased demand for better control
- Improved equipment for process control
- Integration of new control techniques

The first category essentially deals with economic factors, whereas the second and third are related to technological factors affecting hardware and software developments respectively.

The economic factors influencing the developemnt of distillation control have played increasingly important roles. Since the 1970's the cost of energy has made it imperative to design control strategies which minimize energy costs. Shinskey (1984) places great emphasis on the objective of energy conservation, citing a report which concludes that energy is commonly wasted through heat loss to atmosphere, low tray efficiency, excessive reflux, poor selection of feed point, poor design of heat exchange equipment and column designs with insufficient trays. Better control cannot necessarily remedy all of these problems, but it can provide the maximum energy efficiency given the existing equipment. Heat integration within plants has also become an issue of increasing interest. Tyreus and Luyben (1976) published one of the key papers dealing with control of heat integrated columns.

Energy costs are the major operating cost of a distillation unit. A drive to reduce capital plant investment has also played a role in the design of distillation control schemes. Lower capital investment means that towers are designed closer to specifications. Whereas in the past columns were designed with a safety factor of additional trays, this practice has declined with the computer design methods now in use. The computer designed columns require more stringent controls than did earlier designs (Tolliver and McCune, 1978).

A third cost-related factor is that today's specialized markets have led to large price differentials based on product quality. Product specifications are often more demanding and it is necessary that there be few excursions from these specifications if a price penalty is to be avoided. The alternative for off-spec product is to rerun it, in which case the penalty is paid in operating costs. In an interesting example of the benefits obtained due to improved control, Bojnowski *et al.* (1975) summarize savings due to meeting product specification, reducing heat loss, reducing manpower requirements and improving performance so that upstream operations were debottlenecked.

Technological advances have played an important role in the development of distillation control. Buckley (1983) calls attention to one major factor - instrumentation. Early column operators did not have the benefit of automatic controls and valves. Control strategies were necessarily simple. Development of improved pneumatic controllers and transmitters in the period 1945-1960, as well as the introduction of on-line analyzers in about 1950 paved the way for more complex control systems. Electronic analog controllers were developed starting in the mid 1950's. Initially they had less flexibility than the existing pneumatics, but by the early 1970's the two types of controllers were fully competitive. Distributed digital control systems arrived in the late 1970's, adding a further dimension to plant control. The recent development of "smart" controllers and instrumentation will no doubt increase opportunity for complex control strategies as the instruments are less sensitive to ambient conditions, require less maintenance and are in some cases capable of multiple functions.

Closely related to the development of improved instrumentation is the development of computer systems. Early reports of the use of control computers for optimization were contributed by Johnson *et al.* (1964) of Phillips Petroleum. Buckley (1983) reports that computers in the 1960's and 1970's were mainly used for data logging and supervisory control. Improvement in computer reliability, memory and speed have led to greater dependence on computer control. Using computers, processes may be run much closer to constraints then is otherwise possible (Burkett, 1981). Computer control systems marketed today offer great flexibility and, although some innovative applications have been reported (e. g. Brooks and Nazer, 1985), there is no doubt that most are not documented in the open literature.

Last, but not least, developments in control theory have played a tremendous role in the development of distillation control strategies. For example, in the field of multivariable control theory, work on steady state and multivariable frequency domain methods of interaction analysis have implications on distillation control. McAvoy and co-workers have expanded on Bristol's relative gain array method to refine interpretation of the relative gains and to develop a measure of interaction in the presence of disturbances (McAvoy, 1983; Stanley *et al.*, 1985). Multivariable frequency domain methods for interaction analysis have been summarized by MacFarlane (1979) and more recently by Jensen *et al.* (1986) who present a critical review of a variety of interaction measures. An example of an industrial application of the inverse Nyquist array method was presented by Tyreus (1979). Applications of nonlinear and adaptive control theory are also beginning to be reported and it is likely that, in some form, they will eventually become accepted into the mainstream of distillation control. Some of these applications will be discussed later.

1.2.2 Conventional Control

For the purposes of this study, the term "conventional" control is defined as any feedback control strategy which can be implemented without computer support. Fauth and Shinskey (1975) consider this to be the level of "basic regulatory controls" and suggest that it should be part of an extended hierarchy of controls. Similarly, Rademaker *et al.* (1975) designate this as the level of "basic controls" which may or may not be satisfactory without the addition of "extended control schemes". Tolliver and

McCune (1978) define a "basic control scheme" as a pressure control scheme and a composition control scheme.

Classification of conventional control schemes is made difficult by the fact that no unifying nomenclature exists. However, conventional control strategies can be considered under the following headings:

- Mass Balance Control
- Pressure Control
- Quality Control

These categories will be discussed individually, although an overall conventional control scheme must consist of element(s) from each. Table 1.3 summarizes some of the interpretations and definitions used in the literature corresponding to mass balance schemes. Table 1.4 fulfils the same function for pressure control, and Tables 1.5 and 1.6 are concerned with quality control.

In this chapter and throughout the rest of this work, control variable pairings will be represented as ordered pairs. The first element refers to the manipulated variable and the second to the controlled variable. Hence (D,L_D) refers to a control scheme where distillate is manipulated to control the overhead accumulator drum level. A summary of the symbols for the control variables is given in Table 1.2 and in the Nomenclature section.

Table 1.2
CONTROL VARIABLE SYMBOLS

B	bottom product rate
C	condenser duty
D	liquid distillate rate
F	feed rate
L_B	column base surge level
L_C	condenser level (flooded condenser)
L_D	accumulator level
P	column pressure
Q	product quality
Q_B	bottom product quality
Q_D	top product quality
QR	reboiler duty
R	reflux rate
V_D	vapour distillate rate

Mass Balance Control

Mass balance control is defined here as that part of an overall control scheme designed to ensure that, on average, the material balance around the column closes. As shown in Table 1.3, other designations used to describe this concept are material balance control and level control. In some cases the designated scheme is designed for overall control of the column whereas in others it is designed as an element of the overall scheme. The latter meaning is adopted here.

Several comments are appropriate in relation to Table 1.3. Buckley *et al.* (1985) state that the functions of material balance controls are threefold:

- To maintain inventories between upper and lower constraints.
- To maintain an average balance between inflow and outflow.
- To ensure smooth and gradual changes in flow rates.

They note that this can be achieved either in the direction of flow (which corresponds to adjusting product rates to reflect changes in the feed rate), or against the direction of flow (which corresponds to adjusting the feed flow rate to meet desired product rate or other downstream requirement). Control in the direction of flow is most common and most authors rule out the possibility of

Table 1.3

MASS BALANCE CONTROL SCHEMES

Reference	Title of Scheme	Scheme
Boyd (1948a,b)	Material Balance Control - composition control scheme to be used if there is insufficient temperature gradient for temperature feedback	$(B,\frac{B}{F})$, (QR,L_B), (R,R), (D,L_D) Setpoint for $\frac{B}{F}$ control would be determined based on laboratory analysis of product stream.
Buckley (1978) Buckley et al. (1985)	Material Balance Control -possible in direction of flow or in direction opposite to flow -former more common since products are usually "demand" stream -latter more stable, smaller vessels required	Three schemes possible in direction of flow: 1: (D,L_D), (B,L_B) 2: (D,L_D), (QR,L_B) 3: (R,L_D), (B,L_B) Scheme 1 is preferred in the absence of other considerations such as small product streams. Scheme 2 is subject to "many control difficulties" due to base level control via boilup.
Bojnowski et al. (1975)	Direct Material Balance	Product rate manipulated to control composition
Rademaker et al. (1975)	Mass Balance Control -keep D, F, B constant or in a constant ratio -can be used if feed is constant or contains a constant amount of top or bottom product	The authors give an extensive listing of feasible schemes in three categories: 1. Feed and distillate on flow control 2. Feed and bottoms on flow control 3. Distillate and bottoms on flow control Choice depends on particular column. For general case, feed and distillate on flow with: (B,L_B), (C,P), (R,L_D)

Table 1.3 (continued)

Reference	Title of Scheme	Scheme
Ralston (1983)	Material Balance (Level) Control	One product stream controls that stream's composition, the other and reflux or heat input control base and accumulator level
	Indirect Material Balance Control	Reflux or reboiler duty is used to control a product composition and the product rates are used to control levels
Shinskey (1984)	Closing Material Balance	Close using the largest, most variable stream. Possible schemes: (B,L_B), (D,L_D) (B,L_B), (R,L_D) (QR,L_B) or (R,L_B), (D,L_D) (F,L_B), (D,L_D) or (R,L_D) or (QR,L_D)
	Direct Material Balance	Scheme in which a product is manipulated to control a composition
Tolliver and McCune (1978)	Material Balance Control -manipulation of distillate to feed ratio to control the composition of the most valuable product	A. Feed and Heat Input on Flow Control: 1. DIRECT: (D,Q), (B,L_B), (R,L_D) 2. INDIRECT: (D,L_D), (B,L_B), (R,Q) B. Feed and Reflux on Flow Control: 1. DIRECT: (D,L_D), (B,L_B), (QR,Q) 2. INDIRECT: (D,L_D), (B,Q), (QR,L_B)

manipulating feed rate (e. g. Tolliver and McCune, 1978). Others (e. g. Rademaker *et al.*, 1975) indicate possible control strategies involving feed manipulation, but note that these cannot be used unless the final product rate is adjusted independently.

Buckley *et al.* (1985) appear to have misinterpreted at least the most recent edition, (1984), of Shinskey's book on distillation control. They claim that he refers to material balance control as the particular scheme: (R, L_D), $(\frac{D}{F}, Q)$. He in fact labels this as a direct material balance scheme since a product flow is manipulated to control a product composition.

Choice of a material balance control scheme must be made in light of several factors:

- Size of and constraints on manipulated variables:

  The largest, most variable stream should be used to close column material balance (Shinskey, 1984). Rademaker *et al.* (1975) consider this factor in terms of using schemes with distillate on flow control only if the ratio of bottom product to feed flow, $\frac{B}{F}$, is not small. Similarly, they use schemes with bottoms on flow control only if the ratio of top product to feed flow, $\frac{D}{F}$, is not small.

A stream recognized as a column bottleneck should not be used as a manipulated stream (Rademaker *et al.*, 1975).

- Interaction between loops:

  The failure of one loop should not threaten the operation of other loops. Rademaker *et al.* (1975) give as an example a scheme with feed and bottoms on flow control and with condensate receiver level controlled by distillate while base level is controlled by condenser duty. Column pressure is controlled by reboiler heat input. (i. e. (D,L_D), (QR,P), (C,L_B)). If the open loop pressure response to an increase in reboiler heating is not positive, then the sign of the pressure response will depend on whether or not base level were controlled. (See inverse response discussion below and in Section 1.1.5).

- Frequency and type of disturbance expected:

  For example, as stated by Rademaker *et al.* (1975), pressure should be controlled by reboiler heat input if large, fast disturbances in that variable are likely.

- Design constraints of column internals:

  The operating window of the trays should be considered (Rademaker *et al.*, 1975). If the trays are closer to weeping than to flooding, then it is more important to control column vapour flow closely than it is to control column liquid flow.

- Interaction between material and energy balances:

  Tolliver and McCune (1978) state that their scheme designated as A1 in Table 1.3 has the smallest amount of interaction between energy and material balance of the schemes they list, whereas scheme B1 has the greatest amount of interaction. Shinskey (1984) advocates a relative gain analysis of all feasible schemes in order to choose that with the least interaction.

- Inverse response in base level loop:

  As noted in Section 1.1.5, inverse response is possible when base level is controlled by reboiler heat input. All of the authors referenced (with the exception of Boyd (1948a,b)) note the possibility of nonminimum phase behaviour. Unless other considerations outweigh this factor, schemes with the undesirable pairing should be avoided. It should also be noted that inverse response of low boilers in the bottom product stream is also possible. Rademaker *et al.* (1975) recommend ruling out these pairings if the open loop response of column pressure to an increase in boilup is negative or zero.

Pressure Control

Many discussions of distillation control strategies are based on the assumption of ideal pressure control using

Table 1.4

PRESSURE CONTROL SCHEMES

Reference	Title of Scheme	Scheme
Buckley (1978) Buckley et al. (1985)	Considered as part of material balance control	Averaging pressure controls rather than tight controls are recommended. Control P via 1. vent and inert gases (V_D,P) 2. flooded condenser (L_D,P) 3. cooling water (C,P) Control ΔP via reboiler heating (QR,ΔP)
Shinskey (1984)	Closing Energy Balance (Inventory Control)	Exact pressure control required for temperature feedback control. Control P to minimum feasible value. Floating pressure control recommended. Schemes: (C,P) or (QR,P) or (V_D,P)
Rademaker et al. (1975)	Considered as part of mass balance or quality control	Schemes: (C,P) or (QR,P) Use reboiler heating only if open loop response of pressure to an increase in reboiler heating is positive.
Tolliver and McCune (1978)	Pressure Control	(C,P) assumed

condenser duty (e.g. Tolliver and McCune, 1978; McAvoy and Weischedel, 1981). This might lead one to imagine that pressure control is an area of common ground among distillation control experts. However, a survey of recent distillation control reference books uncovers some differences of opinion. (See Table 1.4). Buckley and co-workers (1985) state that pressure control should be of the "averaging" type since abrupt increases or decreases in column pressure could cause dumping or flooding respectively. On the other hand, Shinskey (1984) emphasizes that pressure control is more demanding than level control and must be exact in the common case of temperature feedback control. At the same time, Shinskey advocates floating pressure control as will be discussed below. Authors also differ in the way they classify pressure control. Some (e. g. Rademaker *et al.*, 1975) do not consider pressure control explicitly, but class it only as part of an overall scheme. It has been separated here for two reasons. First, as a category it can conveniently be set aside if ideal pressure control is to be assumed. Second, the separation facilitates comparison of the pressure control schemes suggested in the literature.

As noted by Shinskey (1984), pressure control can be considered as energy balance control. Variations in the energy balance of a column alter the vapour-liquid equilibrium in the tower, hence changing the column pressure.

As can be seen in Table 1.4, three manipulated variables are suggested for pressure control: vent gas or vapour distillate; condenser duty; and reboiler duty. Control with reboiler heat input raises the concerns about inverse response which were discussed in the previous section. For control via vent gas or vapour distillate there must be sufficient gas flow. In some cases it might be necessary to add inert gas to blanket the accumulator and permit better control (Nisenfeld and Seeman, 1981). Control by manipulation of coolant (e. g. cooling water) flow is not generally acceptable (Buckley *et al.*, 1985; Shinskey, 1984). This scheme was once quite common, but due to fouling and corrosion problems at low flow rates it is now considered undesirable.

It is, however, possible to control column pressure with condenser duty indirectly. As noted above, Shinskey (1984) recommends floating pressure control. Using this philosophy, the condenser operates as efficiently as possible at given ambient conditions (Fauth and Shinskey, 1975). This ensures that the column operates at the minimum pressure constraint for the tower which, as noted by Shinskey (1984), is determined by

- Local ambient conditions
- The range of temperature variations for water cooled condensers
- The amount of non-condensables in the feed

- Tray efficiency variation with pressure

Problems due to floating pressure control are that temperatures in the column will vary and tray operating limits may be violated. Buckley (1983) notes that column temperatures and pressures should be allowed to vary rather than being held constant. Shinskey (1984) recommends using pressure-compensated temperature measurements. Both authors recommend the use of constraint (override) controls to avoid working outside the operating window of tray efficiency.

Flooded condenser operation closes material and energy balances of the column simultaneously (Shinskey, 1984). Opinions are divided as to whether or not this mode of operation is recommended. Nisenfeld and Seeman (1981) recommend the scheme, whereas Fauth and Shinskey (1975) do not. Buckley *et al.* (1985) recommend it for some cases, noting that control is simplified but may result in sluggish performance.

Single Quality Control

Although most distillation control literature is aimed at dual composition control, the majority of columns in industry have control systems designed for single composition control only (Buckley *et al.*, 1985). In these cases, it is usually reflux or boilup which is the

Table 1.5

SINGLE QUALITY CONTROL SCHEMES

Reference	Title of Scheme	Scheme
Rademaker et al. (1975)	Direct Quality Control	Four possibilities given. "Best" two: 1. (D,L_D), (B,L_B), (QR,Q), (C,P) 2. (D,L_D), (B,L_B), (R,Q), (C,P)
	Indirect Quality Control	Six possibilities given. "Best" three: 1. (D,Q), (B,L_B), (QR,P), (R,L_D) 2. (D,Q), (B,L_B), (C,P), (R,L_D) 3. (D,L_D), (B,Q), (QR,L_B), (C,P)
Ralston (1983)	Energy Balance Control	Reflux or heat input manipulated to control a product composition (i. e. (R,Q) or (QR,Q))
Shinskey (1984)	Composition Control	Single composition control is not considered except by default for the case when degeneracy prohibits decoupled dual composition control. Single composition control is also considered in relation to feedforward control.
Buckley (1978)	Product Quality Control	Overhead composition controlled by manipulating reflux. Bottom composition controlled via heat input.

manipulated variable as can be seen from Table 1.5. In designing a single composition control scheme the following factors must be considered:

- Type of quality measurement
  - composition
  - temperature
  - pressure corrected temperature
  - vapour pressure
  - differential temperature

- Location of measurement sensor

- Type of feedback controller
  a. proportional-integral
  b. proportional-integral-derivative

The first two of these issues are discussed in Section 1.2.4. As far as the choice of controller is concerned, derivative mode may be added provided the measurement signal is not noisy (Shinskey, 1984). However, most feedback composition controllers are of the proportional-integral type (Buckley *et al.*, 1985).

Dual Quality Control

Dual quality control of distillation columns has been the subject of much recent discussion. Relatively few columns are currently controlled to two product specifications but significant credits can be obtained if both products can be reliably controlled. As noted by Bartman (1981), the dual composition problem becomes more important as reboiling becomes more expensive, especially if top and bottom products have the same value. Where conventional control (in the sense of this work) is to be used, the potential for dual composition control is limited. Most authors, notably Shinskey (1984) and McAvoy (1983), base their approach on Bristol's relative gain array (RGA) and related interaction analysis. This method is now applied in virtually all documented studies (e.g. Bojnowski *et al.*, 1975; Ralston *et al.*, 1985; Frey *et al.*, 1984). A summary of the method is covered in Section 5.4.2. For the purposes of this section, it is the feasible control combinations which are of interest. Figure 1.1 is based on a worksheet used by Shinskey (1984) for control system synthesis with nomenclature altered to agree with that used in this work.

Shinskey rates the control of top product composition using reflux ratio and bottom product composition using boilup as the most common dual composition control scheme. Table 1.6 lists Shinskey's basic dual composition control schemes including the mass balance and pressure controls

MANIPULATED VARIABLE FOR
DISTILLATE COMPOSITION CONTROL

MANIPULATED VARIABLE FOR BOTTOMS COMPOSITION CONTROL	Distillate	Reflux	Reflux/Distillate	Distillate/Overhead Vapour	Distillate/Reflux
Distillate	X			X	X
Bottoms	X				
Boilup					
Boilup/Reflux					
Boilup/Bottoms					
Boilup/Distillate		X	X	X	X
Boilup/Reflux		X	X	X	X

Figure 1.1

VARIABLES FOR COMPLEX DUAL QUALITY CONTROL required to accompany them. He also recommends variations on these schemes which involve cascading the ratios of manipulated variables shown in Figure 1.1. Shinskey admits that the more complex schemes add to hardware costs and decrease the ease of understanding of the control strategy, but states that they offer some improvement in steady state relative gain and reduce delays in the system (Shinskey, 1984).

The schemes listed in Table 1.6 are "optimal" in the sense of using the most favourable steady state relative gains. Dynamic considerations can not be ruled out. (e. g. Roat *et al.*, 1986) so that variations such as using reflux as opposed to reflux ratio to control top composition in Shinskey's SB configuration may be better than the "optimal" structure.

1.2.3 Advanced Control

Based on the definition of conventional control presented in Section 1.2.2, "advanced control" is defined as any control strategy more complex than conventional feedback control. Rademaker *et al.* (1975) consider a similar class of control strategies which they designate "extended control schemes". These consist of accessory feedback control schemes (e. g. control of latent heat, combustion heat or internal flows); ratio control; feedforward control; dual quality control; control of tray loading; and optimizing control. The category, then, can be seen to cover a wide

Table 1.6

DUAL QUALITY CONTROL SCHEMES

Shinskey Title	Strategy	Comments
SV	$(C,P)\ (R,L_D)\ (B,L_B)$ $(\frac{R}{D},Q_D)\ (QR,Q_B)$	Simplified form of SV/B which Shinskey judges the most generally applicable.
DV	$(C,P)\ (R,L_D)\ (B,L_B)$ $(D,Q_D)\ (QR,Q_B)$	May have sluggish response. Use for high reflux columns with high purity bottoms.
SD	$(C,P)\ (QR,L_D)\ (B,L_B)$ $(\frac{R}{D},Q_D)\ (D,Q_B)$	Best for high reflux towers with top product purer than bottom product. May need to detune top composition controller. Not common.
SB	$(C,P)\ (D,L_D)\ (QR,L_B)$ $(\frac{R}{D},Q_D)\ (B,Q_B)$	Use if separating a small amount of heavy contaminant from a high purity product.

spectrum of control strategies. For the purposes of this section, those falling under the following headings will be briefly discussed:

- Feedforward control
- Decoupling control
- Adaptive control

Feedforward control is widely used in industry. Decoupling control applications are also quite common and the term has been taken here to include any multivariable control scheme designed to minimize interaction effects. There is some overlap between this category and that of adaptive control as many adaptive schemes are also multivariable and also minimize interaction between control loops. Adaptive control is taken here to include any scheme in which parameters are automatically varied. Applications of adaptive schemes are expected to provide considerable benefits in industrial applications.

Before implementing advanced control techniques certain tradeoffs must be made. Each application requires considerable development work and this must be weighed against the potential credits to be obtained for that single implementation to determine whether the work is justified (Pearson, 1984). The price difference between conventional and advanced control was once dominated by hardware costs, but the dominating factor is now much more likely to be the cost of application engineering work, particularly the development of adequate process models (Rijnsdorp and Seborg, 1976; Pearson, 1984). In addition to the cost-benefit analysis required for each application, it is necessary to determine whether the tools, hardware and software, are available.

The sections which follow summarize some applications and recommendations discussed in the literature for feedforward, decoupling and adaptive control.

Feedforward Control

Opinions on the use of feedforward control have changed within the past twenty years. There have been progressively more applications and with progressively more success. Tolliver and Waggoner (1980) quote sources approximating the number of feedforward applications in the United States and Canada at 150 at that time. Buckley *et al.* (1985) list as the benefits of feedforward control:

- Compositions may be more tightly controlled to setpoint than is possible with feedback control alone.
- Feedforward control poses none of the stability problems common with tightly tuned feedback controllers.
- Maximum column capacity is increased using feedforward control since changes in manipulated variables are smaller. As a further result the trays are less likely

to weep or dump.

Table 1.7 summarizes some documented applications and Table 1.8 lists recommendations given in recent distillation control literature.

Decoupling Control

Decoupling, or multivariable, control techniques are appropriate for distillation column control because they provide a means to handle the interaction inherent in distillation processes. Multivariable control techniques rely on simple process models obtained either from linearized mechanistic models or from frequency response relations. Multivariable controllers may be designed either using a decoupling approach or using a frequency domain approach such as the characteristic loci method. Wood and Berry (1973) documented a successful application of the decoupling approach while some later applications have included multivariable frequency domain techniques (e. g. Tyreus, 1979). A survey of experimental applications of multivariable control includes industrial and pilot scale work on distillation columns prior to 1976 (Rijnsdorp and Seborg, 1976).

The entries in Table 1.9 summarize selected recent contributions to the literature on applications of decoupling control to distillation columns. In addition, many of the adaptive control schemes discussed later in this

Table 1.7

APPLICATIONS OF FEEDFORWARD CONTROL

Reference	Comments
Wade, Ryskamp and Britton (1977)	Feed rate and temperature measured for feedforward control APPLICATION: crude tower
Luyben (1969a)	For feed composition disturbances, temperature feedback setpoints must be adjusted as well as reflux, boilup. Addition of feedforward control reduced interaction in feedback loops. APPLICATION: digital simulation, 20 tray binary column
Roach (1970)	Feed composition sets reflux and bottoms rates. Dynamic compensation was included. Application was not entirely successful due to problems with analyzer and with dynamics of a direct fired reboiler. APPLICATION: debutanizer tower
Readshaw and Boyd (1974)	Steam controlled on flow with trim controller using feedforward terms from a) column feed rate b) internal reflux rate c) steam pressure. APPLICATION: methanol refining column
Oglesby and Lupfer (1962)	Feed enthalpy computer used to break interaction due to a feed-bottoms exchanger. APPLICATION: debutanizer and partial depropanizer tower
Dobson (1960)	Feed enthalpy control dictates separation of a binary mixture APPLICATION: simulation study

Table 1.8

LITERATURE RECOMMENDATIONS FOR FEEDFORWARD CONTROL

Reference	Comments
Rademaker et al. (1975)	Restrict feedforward control to that based on feed rate. Combine with feedback quality control. Composition dynamics are slower and can be dealt with using feedback control alone.
Buckley et al. (1985)	Use feedforward for fast, approximate control and feedback for long-term, accurate control. Generally do not need feedforward based on feed composition. Feedforward schemes based on ratio controls are recommended: e. g. in direction of flow (D,L_D), (B,L_B), $(\frac{R}{F},Q_D)$, $(\frac{QR}{F},Q_B)$
Deshpande (1985)	For single composition control: use feedforward control on reflux or boilup. For dual composition control: use feedforward and feedback for one composition loop with feedback alone for the other.
Shinskey (1984)	Many of this author's optimal structures are recommended in conjunction with ratio feedforward action.

section should be considered as further examples of multivariable control.

Adaptive Control

Adaptive control applications to distillation column control are of increasing interest as hardware limitations are diminished. Adaptive techniques have particular potential for distillation applications because the strategies are appropriate for nonlinear processes and those in which process parameters and operating conditions are time varying. The control techniques themselves can vary from relatively simple adaptive gain algorithms to much more complex schemes requiring considerable computation and computer memory.

Tables 1.10 through 1.12 summarize some recent reports of applications of adaptive control techniques to distillation in simulation, in experimental work on pilot scale units and in industrial environments. The entries in Table 1.10 are concerned with applications of self-tuning control while those in Table 1.11 deal with inferential control applications and other adaptive control applications are covered in Table 1.12. The lists are by no means exhaustive, but do serve to indicate that there is an active interest in the use of adaptive control for control of distillation processes.

Table 1.9

SELECTED APPLICATIONS OF MULTIVARIABLE CONTROL

Reference	Comments
Schwanke et al. (1977)	Application of classical decoupling and characteristic loci methods for multivariable control of a simulated binary column. Noninteracting control was not achieved using the characteristic loci method, likely due to inexperience with the method.
Takamatsu et al. (1981)	Application of "GG-pseudo-band method" (an extension of the inverse Nyquist array method) to a pilot scale binary column. Use of simulation recommended since controller design involved some trial and error and judgment work. Performance was degraded by sensitivity to noise.
Thompson (1982)	Application of a multivariable PID controller with decoupling based on open loop step responses. Transfer function model used for distillation simulation. Reasonable decoupling was obtained
Karim and Lee (1983)	Study of the performance of several multivariable controller designs for a system with changing process parameters. Decoupling and optimal state feedback provided inadequate performance while performance with pole assignment control was better but deteriorated when parameters changed.

Table 1.10

APPLICATIONS OF SELF-TUNING CONTROL

Reference	Type of Application	Comments
Dahlqvist (1980)	- simulation - experimental (pilot scale)	Good performance obtained provided that tuning factors were properly adjusted.
Morris et al. (1982)	- simulation - experimental (pilot scale)	Disturbance feedforward polynomial identification was included to avoid problems with load disturbance rejection. Q weightings were incorporated and multirate sampling permitted good dual quality control.
Chien et al. (1983)	- simulation	Application for a binary column simulation. STC using extended least squares was successfully applied with multirate sampling and multiple time delays permitted.
Brooks et al. (1983)	- experimental (industrial column)	STC was used since fixed parameter deadtime compensation had been unsatisfactory. Good performance was obtained for single quality control.
Chien et al. (1985)	- experimental (pilot scale)	Performance was found to depend on the tuning of the estimation algorithm, but dual quality control was better than was possible with conventional PI controllers.

Table 1.11

SIMULATION STUDIES OF INFERENTIAL CONTROL

Reference	Comments
Cviklinski and Brosilov (1977)	Inferential single quality control was attempted but failed because of nonlinear behaviour. Performance was improved by reassigning control variables but an offset was observed and was said to be due to interactive effects from unmeasurable disturbances.
Joseph and Brosilov (1978a)	Steady state inferential control was studied by developing a steady state estimator and considering steady state control performance for a linearized debutanizer model. Sensitivity to the number of secondary measurements and to coupling between measurements was considered with a trial and error approach used to select the appropriate measurement set.
Brosilov and Tong (1978)	Dynamic compensation in the form of a simple lead-lag network was added to the steady state inferential control system of Joseph and Brosilov (1978a). Single and dual quality control of a linearized depropanizer model were considered and were found to be better than the comparable conventional feedback control.
Joseph and Brosilov (1978b)	Development of optimal and suboptimal dynamic estimators was discussed and the performance of the resulting inferential control schemes tested on a linear input-output model of a multicomponent distillation column. Little benefit was derived from the use of optimal estimators.
Patke et al. (1982)	Inferential control based on the work of Brosilov and co-workers was applied to a depropanizer tower in simulation. Control performance was compared with conventional and parallel cascade control. Settling times were found to be faster with inferential control and less overshoot was observed. Some steady state offset was observed, but it was conjectured that this might not be found to be a problem in experimental work.
Yu and Luyben (1984)	A scheme in which two differential temperatures were used to adjust the setpoint of a temperature feedback controller was found to yield less steady state offset than the inferential control results presented by Patke et al. (1982). No dynamic simulation was performed.
Parrish and Brosilov (1985)	Practical issues involved in implementation of inferential control to a nonlinear autoclave process were discussed.

Table 1.12

OTHER ADAPTIVE CONTROL APPLICATIONS

Reference	Type of Application	Comments
Wiemer et al. (1983)	pilot scale column	MODEL REFERENCE CONTROL SCHEME A fixed gain estimator was used and the controller was said to be more simple than the STC while performance was comparable. Less storage and computational effort were required than were needed for STC.
Barcenas and Alvarez (1983)	simulation	MODEL REFERENCE CONTROL SCHEME Offline parameter identification was used to initialize parameters. Successful dual composition control was obtained with the controller designed to switch to a fixed gain controller when prediction error was within a certain deadband.
Martin-Sanchez and Shah (1984)	pilot scale column	ADAPTIVE PREDICTIVE CONTROL SCHEME MIMO and SISO control outperformed classical techniques.
Gerry et al. (1983)	pilot scale column	POLE-ZERO PLACEMENT SCHEME Dual quality SISO control performance was better than the corresponding PID control performance.

1.2.4 Implementing Distillation Column Control

Most of the considerations regarding distillation column control implementation are common to all process control installations. Some, however, are of special concern for distillation applications. Buckley *et al*. (1985) present a number of practical considerations based on operating experience. The issues which will be considered here are sensor location, the use of analyzers for on-line quality measurements and the design of override (constraint) controls. Proper handling of these issues is integral to good control. They are also issues which may be explored in simulation, making it especially appropriate that they should be discussed here.

Sensor Location

Many criteria have been suggested for determining the optimum control tray for temperature feedback control. In practice, selection of the control point is generally the result of compromise between different criteria (Wood, 1967). Rademaker *et al*. (1975) summarize some of the literature in the area. The majority of the criteria are based on steady state column data (e. g. Tivy, 1948; Wood, 1967; and most of the sources listed by Rademaker *et al*., 1975). Column dynamic effects have also been considered by some authors (Shunta and Luyben, 1971; Tolliver and McCune, 1980; and Rademaker *et al*., 1975).

Steady state criteria may be classed into the following categories:

- profile gradient
- control point temperature sensitivity
- steady state disturbance response

Criteria concerned with the steady state temperature gradient were perhaps the earliest proposed. Boyd (1948a,b) recommends that temperature sensors be located where the steady state temperature gradient is greatest. This selection method is still in use. Buckley *et al.* (1985) state that sensors are typically located by selecting a tray in a region where temperature changes rapidly from tray to tray. Rademaker *et al.* (1975) disagree with this criterion, noting that the gradient is proportional to initial response only and can not take into account the dynamic effects of neighbouring trays. Uitti (1950) also criticizes the use of steady state temperature gradient as a criterion since the gradient depends on the reflux ratio.

Considerations based on steady state disturbance response (i. e. final steady state conditions after a disturbance) are that the temperature at the control point should be correlated strongly with product composition (Shinskey, 1984; Rademaker *et al.*, 1975); that the temperature deviation for step increases and decreases of a given magnitude should be symmetrical and as large as possible (Tolliver and McCune, 1978); that the temperature deviation over a series of simulations varying reflux ratio should be maximized; and that the steady state response should be linear (Buckley *et al.*, 1985). Use of all of these criteria involves parametric column studies. The procedure suggested by Rademaker *et al.* (1975) involves analysis of "quasi-steady state" data to minimize the sum of weighted product composition variation.

Temperatures at the sensor location should be sensitive to key component concentration and insensitive to changes in non-key component concentration. It is this criterion that necessitates moving the control point away from the ends of the tower despite dynamic considerations. Williams *et al.* (1956) note that the sensor must be able to detect variations in the controlled temperature as well as the temperature itself. The size of the "dead zone" in which temperature variations can not be detected may vary with control point.

Dynamic considerations regarding sensor location require that the temperatures at the control point must be responsive to changes in the manipulated variable, but must provide some insulation from effects of feed and reflux enthalpy changes (Shinskey, 1984). Rademaker *et al.* (1975) cite the speed of the control loops as one of the most important criteria for sensor location. This is not purely a function of the number of stages between the sensor and the control valve as the response speed may be affected by other column variables such as pressure drop. Tolliver and McCune (1980) state that their criteria of maximum symmetrical profile response to step changes ensures dynamic response at least as fast as that on any other stage.

All of the above criteria must be balanced to determine the best temperature sensor location. Dynamic simulations serve as a useful tool at the design stage to speed the procedure. Although some *a posteriori* adjustment may be required, consideration of all of the factors addressed here guarantees improvement of the selection procedure relative to the days when Boyd (1948a,b) suggested locating thermowells on every third tray for field testing.

Use of Composition Analyzers

Although temperature measurements provide an indication of the liquid composition, the accuracy of the inferred quality measurement is far from ideal and a direct composition measurement is desirable for control. Periodic laboratory analyses have traditionally been used to improve control as the data can be used to determine updated setpoints. Online analyzers provide more frequent direct composition measurement. Unfortunately, the poor reliablity and high cost associated with analyzers have restricted their use. Literature reports advocating the use of analyzers have suggested that they should be used with safeguards for system integrity in the event of an analyzer failure. Limits to controller output, checks on the rate of change of composition measurements, and the use of feedforward control in addition to feedback control based on the analyzer measurements have all been suggested (Griffin *et al.*, 1978). There is now some evidence that analyzers have improved to the point that current applications are not taking advantage of current technology (Krigman, 1986). An industry opinion survey indicated that performance can be satisfactory if expectations are realistic and if adequate emphasis is placed on preventative maintenance. Resultant savings are obtained both directly and indirectly. Improvements in product quality and yield provide direct benefits, as do reduced operating costs. Indirect credits may be realized when online measurements are used as the basis for advanced control or when the use of analyzers leads to an increased emphasis on preventative maintenance in general (Krigman, 1986). In addition, analyzer costs have been reduced over the years by improvements in technology. Use of distributed analyzer systems can lower costs even more (Yeh, 1986). As the result of these factors, composition analyzers can be economically justified for an increasing number of processes.

The comment about realistic expectations applies to the selection of an appropriate analyzer type and model. Reliability problems can often be attributed to poor matching of analyzer specifications with control requirements. Instrument selectivity, sensitivity, response time, accuracy, range, and repeatability must be appropriate to the application. Installation, sampling systems and sample conditioning also have significant affects on performance (Yeh, 1986).

Gas chromatographs are the analyzers most commonly used for distillation applications. Technological improvements have made possible instruments with an accuracy of 1% of full scale and response times in the order of 30 - 120 seconds (Yeh, 1986). Developments in fiber optics and microelectronics are expected to result in improved sensors and detectors which will further improve composition analyzer accuracy and reliablity (Hirschfeld, 1986).

Constraint Control

Distillation operations must be carried out within an operating window defined by "hard" and "soft" constraints. Hard constraints may not be violated for safety reasons or represent physical limitations (e. g. valve saturation) whereas soft constraints are those which define efficient operating conditions. No practical distillation control system can be considered complete without consideration of the constraints. As a result, the topic of constraint control has been covered in great depth by Buckley *et al.* (1985) and Shinskey (1984). Since a detailed discussion of the design of constraint control systems is beyond the scope of this work, the intent of this section is simply to flag the topic as an important element of distillation control system design.

Constraint and override controls are imposed for the following reasons (Buckley *et al.*, 1985):

- safe, satisfactory column operation

  consider

  - maximum operating pressure
  - condenser and reboiler constraints
  - column flooding limits
  - tray weeping/dumping limits
- startup and shutdown situations
- changes in feed stock or product compositions

The relative importance of these items must be evaluated and an appropriate constraint and override system designed. Buckley (1978) suggests that constraint control design should form the third and final tier of the overall control system design.

Types of constraint control recommended vary from external controller feedback (anti-reset windup) used to eliminate integral action when a hard constraint such as valve saturation is reached (Shinskey, 1984; Buckley *et al.*, 1985); to selective control systems in which high/low signal selectors are used to maintain operation within constraints (Maarleveld and Rijnsdorp, 1970);

to variable structure control systems which often result in the sacrifice of a quality control loop in order to control an important pressure or level (Shinskey, 1984).

2. DEVELOPMENT OF DYNAMIC SIMULATOR

2.1 Introduction

The digital simulation program used in this work was developed by Wong (1985) with a solution procedure based on an earlier program written at Case Western Reserve (Cook, 1980; Ballard *et al.*, 1978).

The model equations will be outlined in Section 2.2 with a discussion of the solution procedure given in Section 2.3. Section 2.4 deals with the structure of the simulator. The final section in the chapter covers modifications made to the simulation package during the course of this work.

2.2 Model Development

The computation involves the solution of a set of ordinary differential and algebraic equations written to describe the dynamic behaviour of a multicomponent plate distillation column. These equations are based on rigorous heat and material balances as described in detail by Rademaker *et al.* (1975). The equations are derived for a general case, so that the program has the flexibility required to describe towers with multiple product streams and/or feeds. This approach permits simulation of complex towers with large numbers of trays and many components which may behave nonideally. The current version of the program is limited to 90 stages and 10 components. The tray equations are written for a general stage which may represent a tray, partial or total condenser or reboiler. Figure 2.1 shows a generalized tray with vapour and liquid sidedraws as well as a feed stream. The sections that follow will outline the material and energy balances for this generalized tray as well as discussing the representation of thermodynamic behaviour of the liquid and vapour streams. A further section deals with the overall balances and the combination of the heat and material balances with pressure drop, efficiency, liquid holdup and heat loss correlations to form the overall column model.

2.2.1 Material Balance Equation

For each stage in the column NC+1 material balance equations may be written where NC is the number of components in the system. This applies regardless of whether the stage represents a tray or the reboiler or condenser. The following assumptions are made in deriving these equations:

- non-reactive mixture
- perfect mixing on all trays
- negligible material holdup in the vapour phase and in the downcomer

Numbering the stages from the condenser as shown in Figure 2.2, the overall material balance may be written as:

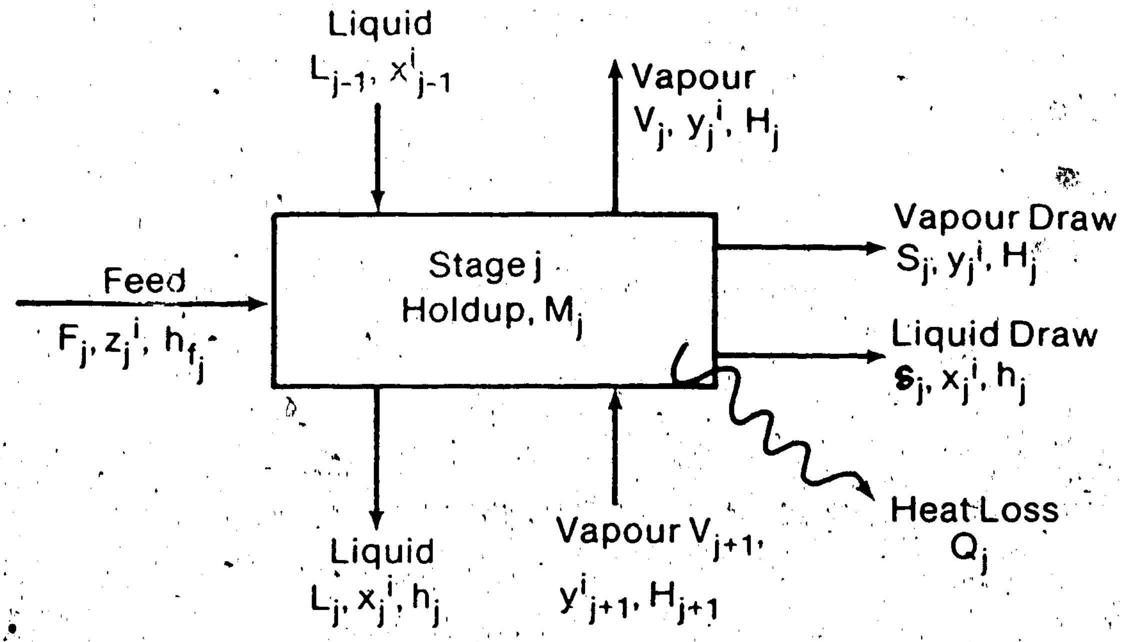


Figure 2.1

DIAGRAM OF GENERALIZED TRAY

$$\frac{dM_j}{dt} = F_j + V_{j+1} + L_{j-1} - (V_j+S_j) - (L_j+s_j) \qquad (2.1)$$

It should be noted that Equation 2.1 becomes an algebraic equation if constant molar holdup is assumed.

A partial material balance may also be written for each component on the stage. Designating the component mole fractions in the liquid, vapour and feed as x_j, y_j and z_j respectively, the balance equation becomes

$$M_j\frac{dx_j}{dt} = F_j(z_j-x_j) + V_{j+1}(y_{j+1}-x_j) + L_{j-1}(x_{j-1}-x_j) - (V_j+S_j)(y_j-x_j) \qquad (2.2)$$

This does not reduce to an algebraic equation under the assumption of constant molar holdup on the tray and must always be solved by integration as discussed in Section 2.3.

A more detailed presentation of the development of these equations is presented by Wong (1985). The intention here is to establish both nomenclature and the assumptions inherent in the simulator as well as those assumptions which may be made at the user's discretion.

2.2.2 Tray Energy Balance

The energy balance of a general stage may be written based on the following assumptions:

- negligible energy and material holdup in the vapour phase.
- negligible energy storage in the tray metal
- negligible energy storage in the downcomer

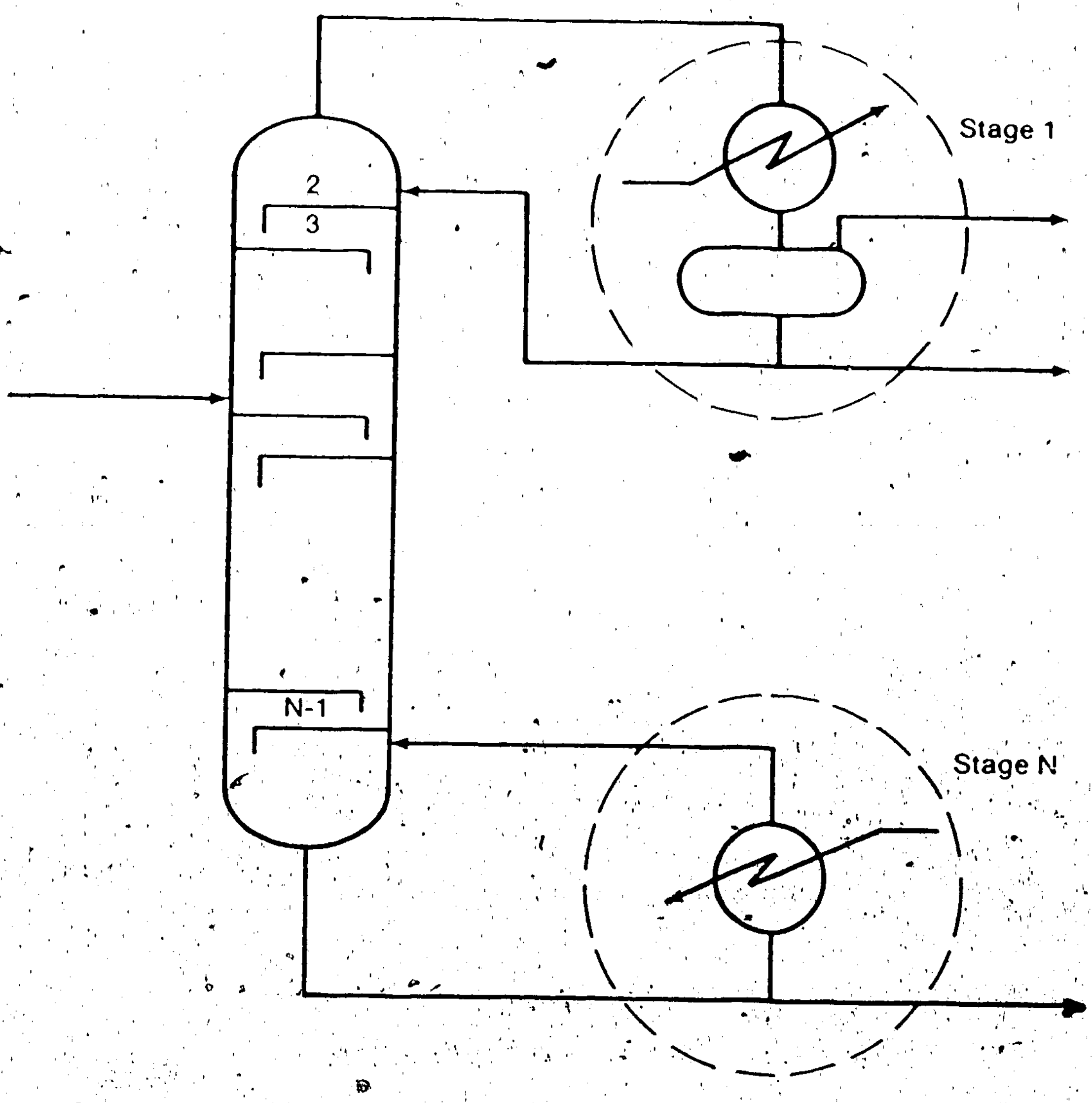


Figure 2.2

TOWER SCHEMATIC

- negligible heat of mixing among species

The resulting equation includes terms describing heat transfer in the form of heat loss to the environment or due to heat exchange in a condenser, intercooler or reboiler. As a generalized stage equation, it applies for a total or partial condenser or reboiler as well as for a tray.

$$M_j\frac{dh_j}{dt} = F_j(h_{fj}-h_j) + Q_j + V_{j+1}(H_{j+1}-h_j) + L_{j-1}(h_{j-1}-h_j) - (V_j+S_j)(H_j-h_j) \qquad (2.3)$$

Equation 2.3 is transformed into an algebraic equation with coefficients which are functions of the heat capacities and vapour and liquid enthalpies of the components

$$E_j = -\alpha_j L_{j-1} + \beta_j V_j + \psi_j V_{j+1} \qquad (2.4)$$

The values of the coefficients E_j, α_j, β_j and ψ_j are given in Table 2.1. The energy balance equations are solved for the stage vapour rates using the Thomas algorithm since the set of equations forms a band diagonal system matrix (Wong, 1985).

2.2.3 Representation of Thermodynamic Properties

In order to deal with both ideal and nonideal components and with data from a wide variety of sources, the simulator is designed to permit flexible representation of thermodynamic data. For example, vapour and liquid enthalpy

Table 2.1

ENERGY BALANCE COEFFICIENTS

$$\alpha_j = h_{j-1} - h_j - \xi_j^1 \qquad (2.5)$$

$$\beta_j = H_j - h_j - \xi_j^2 \qquad (2.6)$$

$$\psi_j = H_{j+1} - h_j - \xi_j^3 \qquad (2.7)$$

$$E_j = F_j[h_{Fj} - h_j - \xi_j^4] - \beta_j S_j + Q_j \qquad (2.8)$$

where
$$\xi_j^1 = \sum_{i=1}^{NC} [\Gamma_{ji}(x_{j-1,i} - x_{ji})] \qquad (2.9)$$

$$\xi_j^2 = \sum_{i=1}^{NC} [\Gamma_{ji}(y_{ji} - x_{ji})] \qquad (2.10)$$

$$\xi_j^3 = \sum_{i=1}^{NC} [\Gamma_{ji}(y_{j+1,i} - x_{ji})] \qquad (2.11)$$

$$\xi_j^4 = \sum_{i=1}^{NC} [\Gamma_{ji}(z_{ji} - x_{ji})] \qquad (2.12)$$

and
$$\Gamma_{ji} = Cp_j \left(\frac{\partial T_j}{\partial x_{ji}}\right) + \left(\frac{\partial h_j}{\partial x_{ji}}\right) \qquad (2.13)$$

data may typically be expressed as a polynomial function of temperature or, alternatively, may be interpolated from available enthalpy-temperature data.

For systems with little deviation from ideal behaviour in the liquid phase equilibrium coefficients are based on coefficient data supplied by the user. For example, the coefficients can readily be handled as polynomial functions of temperature and/or pressure or may be interpolated from experimental data. Many hydrocarbon systems belong to this class. In more complex systems with nonideal liquid phase behaviour, activity coefficients of each component in the mixture must be calculated. Correlations developed for activity coefficient calculation include the Margules equation and the Wilson equation (Smith and Van Ness, 1975). The Wilson equation is used to calculate the activity coefficents in the current version of the simulation program. This requires input of the interaction coefficients used in the equation:

$$\ln(\gamma_i) = 1 - \ln\left[\sum_j x_j \; G_{ij}\right] - \sum_k \left[\frac{x_k \; G_{ki}}{\sum_j x_j \; G_{kj}}\right]$$

where

$$G_{ij} = \frac{\nu_j}{\nu_i} \exp\left(\frac{-a_{ij}}{RT}\right) \qquad (2.14)$$

The interaction coefficients, a_{ij}, are available in the literature for many component pairs. An alternative correlation could also be incorporated into the program by replacement of the relevant program module.

The equilibrium relationship is used in an iterative procedure based on Newton's method to solve for stage temperatures and vapour component mole fractions using the liquid component mole fractions determined by integration of Equation 2.2.

2.2.4 Overall Column Model

The heat and ~~material~~ balances noted above constitute the core of the multicomponent distillation simulation. Other models must, however, be considered to simulate the behaviour of the overall column.

TRAY EFFICIENCY CALCULATIONS

The equilibrium coefficients discussed in Section 2.2.3 relate the vapour composition to the liquid composition on stage if the two phases are in equilibrium. As has been discussed in Section 1.1.1, the stage efficiency is a measure of the approach to equilibrium achieved on a given stage. The dynamic simulator used in this work currently has the following stage efficiency correlation options:

- 100% Efficiency:

  Use of this option generally requires *a priori* approximation of the number of ideal stages required to achieve the separation observed in the actual tower.
- Efficiency correlated with the composition on a given

stage:

This option is most useful when experimental data are available for direct comparison.

Tray efficiency correlations based on Murphree efficiency could also be incorporated in the simulator should this be required.

TRAY HEAT LOSS

Heat loss from the column may be accounted for either by specifying heat transfer coefficients or by specifying a correlation relating heat loss to the composition on a given stage. Heat transfer coefficients may be specified on a tray-by-tray basis or for sections of the column. An ideally insulated column may be assumed, in which case the heat transfer coefficients for all trays are set to zero.

PRESSURE DROP

The user may select a linearized, constant pressure drop option. In this case the pressure at the condenser and reboiler as well as at the bottom and top trays must be specified. Alternatively a variable pressure drop may specified. In this case the pressure drop is calculated based on user-specified tray parameters.

LIQUID HOLDUP

The simulator is written to include several tray liquid holdup options:

- constant molar holdup
- variable holdup calculated using the Francis weir equation and user-specified tray parameters
- variable holdup correlated to column liquid and/or vapour flow rates.

A compromise between the additional accuracy and the additional computational effort of a variable holdup option may be obtained by using a holdup distribution calculated in a preliminary variable holdup case for subsequent constant holdup cases.

2.3 Solution Procedure

Computer processing time requirements for the solution of dynamic multicomponent distillation cases using this simulator vary with

- length of the transient period to be simulated
- severity of disturbance (since a smaller time step is required for the integration when the column conditions change rapidly)
- assumptions made (constant versus variable holdup has a great effect on computational effort)
- selection of integration parameters
- print interval selected

These factors are discussed in greater detail in the simulator user's manual (Carling, 1986).

2.3.1 Methods of Solution

The material and energy balances as well as the condition of equilibrium between vapour and liquid phases on an ideal stage must be solved for each stage in the column. The resulting set of N(2NC + 3) equations has been called the "MESH" Equations (Henley and Seader, 1981).

For a transient case, the MESH equations must be solved at each time step. The composition and liquid rates are first determined. In the case of assumed constant molar holdup on each stage, the liquid rate equation is algebraic. The liquid rate profile is therefore determined at the same time as the vapour rate profile in an iterative procedure.

For the case of variable molar holdup on each tray, however, the liquid profile must be determined by integration of Equation 2.1. Regardless of whether constant or variable holdup is assumed, the composition calculation depends on integrating Equation 2.2.

The essential features of the solution procedure used in the simulator are summarized as shown in Figure 2.3 in the form of a flow chart for the variable holdup case.

2.3.2 Integration Procedure

The integration routine used in the current version of the simulator is the adaptive semi-implicit Runge-Kutta (ASIRK) method proposed by Prokopakis and Seider (1981). Some features of this method have been discussed in Section 1.1.4. The algorithm has an embedded error estimate

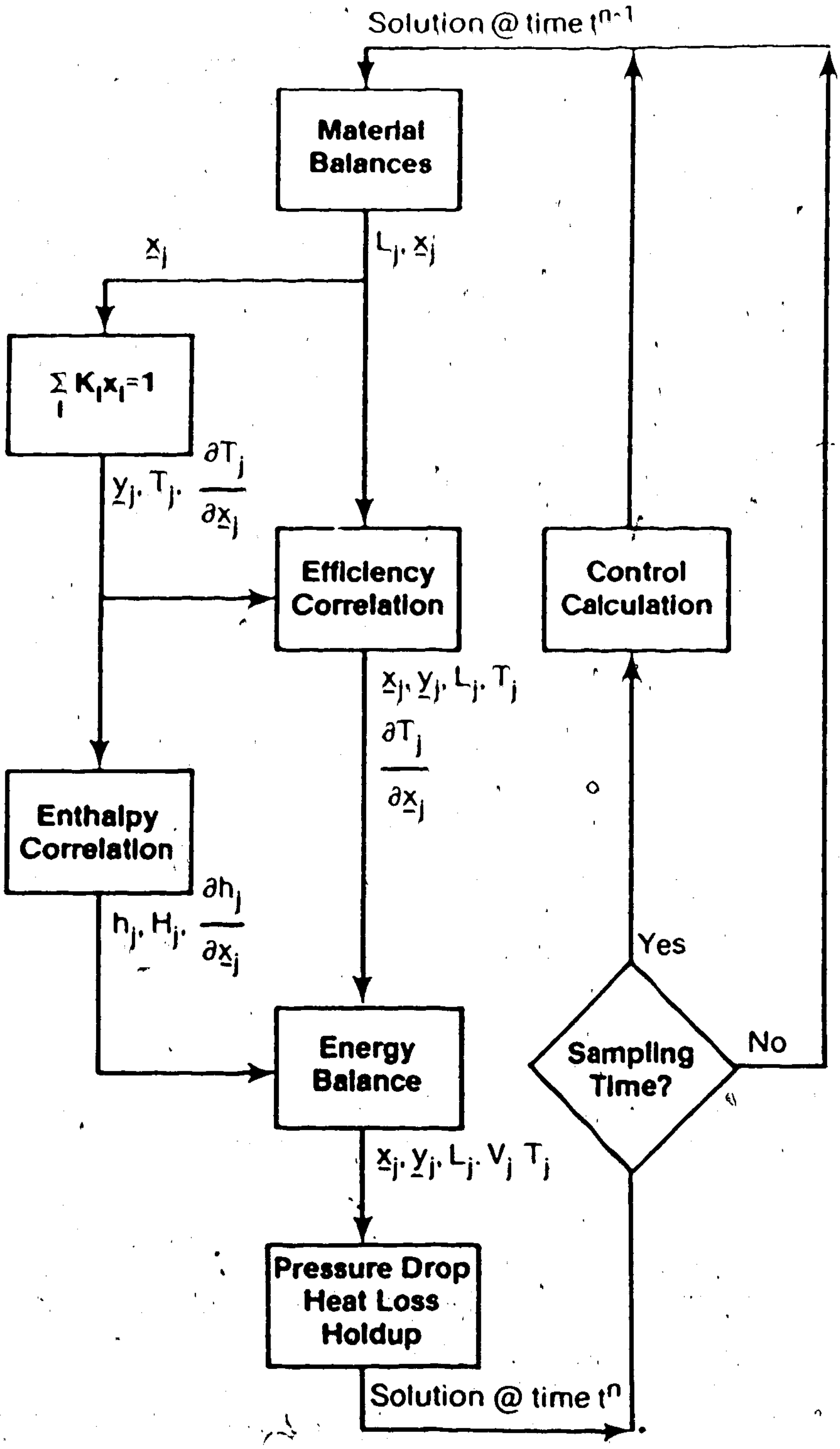


Figure 2.3

SOLUTION PROCEDURE WITH VARIABLE HOLDUP

and the integration step size is controlled based on an estimate of the degree of stiffness of the set of equations. The calculations required in the procedure are summarized in Table 2.2.

The step size control strategy described by Equation 2.21 is adopted from the work of Ballard *et al.* (1978). It was selected in place of the strategy suggested by Prokopakis and Seider since the latter scheme is computationally complex (Wong, 1985).

The estimate of the pseudo-eigenvalue, as described by Equation 2.20 is based on a first order approximation of the derivative $\frac{\partial y_j}{\partial y_s}$. Although Prokopakis and Seider (1981) found that the first order approximation occasionally did not provide sufficient accuracy, it has not presented any problems in this work. Use of the first order approximation simplifies the calculations.

Certain user-supplied parameters affect both the accuracy and the efficiency of the integration through the control of the integration step size. Allowable minimum and maximum step sizes must be provided as must the step size control parameter, σ. Using the relation defined by Equation 2.23, σ controls the sensitivity of the method to the estimate of stiffness provided by the pseudo-eigenvalue of the stiffest equation in the set, λ_s. A certain amount of judgement must be applied when selecting σ since its magnitude represents a trade-off between the speed and accuracy of the resulting solution.

Table 2.2

ASIRK INTEGRATION PROCEDURE

- Calculation of Runge-Kutta Increment Functions:

$$k_1 = hf\{y^n\}\ [I-haJ\{y^n\}]^{-1} \tag{2.15}$$

$$k_2 = hf\{y^n\}+bk_1\ [I-haJ\{y^n\}]^{-1} \tag{2.16}$$

where $a = \dfrac{1 + [1 - 0.5(1 - \gamma_\infty)]^{1/2}}{(1 - \gamma_\infty)}$

$b = \dfrac{1}{3(0.5 - a)}$

- Estimation of Local Truncation Error:

$$e = w(k_2 - k_1) \tag{2.17}$$

where $w = 3(0.5 - a)(a^2 - 2a + 0.5)$

- Criterion for Accepting Step:

$$\sum_{j=1}^{N} \left| \frac{e_j}{y_j^{\,n}} \right| < 4 \cdot N \cdot \sigma \tag{2.18}$$

where N = number of equations in the set

- Integration for Accepted Step:

$$y^{n+1} = y^n + w_1 k_1 + w_2 k_2 \tag{2.19}$$

where $w_2 = 3(0.5 - a)^2$ and $w_1 = 1 - w_2$

- Determination of Pseudo-Eigenvalue:

$$\hat{\lambda}_s = \frac{1}{ha}\left[1 - h\,\frac{f_s\{y^n\}}{k_{1s}}\right] \tag{2.20}$$

- Calculation of New Step Size:

(i) If step has been accepted:

$h^{n+1} = h^n[\dfrac{\sigma}{e_t}]^{1/2}$ provided that $0.25 \le \dfrac{h^{n+1}}{h^n} \le 2.$

(ii) If step has been rejected:

$$h^{n+1} = \frac{h^n}{2} \tag{2.21}$$

Table 2.2 continued

- Calculation of Limiting Characteristic Value

$$\gamma_\infty = \frac{A}{B + (h\lambda_s)^2} + \frac{C}{D + (h\lambda_s)} \tag{2.22}$$

where $A = -4.9921$

$B = 21.1642$

$C = 0.5287$

$D = -0.6889$

provided that $-0.99 \le \gamma_\infty \le 0$.

2.4 Program Structure

The dynamic simulator, known as DYCONDIST, has been written with a modular structure to facilitate both maintenance of the code and future modifications to the code. The current version has about 60 subroutines and about 4500 lines of source code. The code is written in Fortran 77 with object code stored in a subroutine library. Full documentation of the simulator is provided in a user's manual (Carling, 1986).

To make additions and modifications to the program easier, a program structure chart has been drawn up *a posteriori*. The chart and corresponding interface table are included in the DYCONDIST user's manual (Carling, 1986). An additional table in the manual defines common block variables.

2.5 Modifications to Dynamic Simulator

The basic design of the simulator was discussed by Wong (1984) and the reader has been referred to that work for details on simulator development. Some features have been added over the course of this work and these will be outlined here.

2.5.1 Input Generator

An interactive program generating the formatted input to the simulator has been written. The routine is designed for the infrequent user and as a result includes extensive prompting messages. Some checks on the input data are incorporated to avoid data which are out of range or which specify an infeasible column or column configuration. Much of the data is echoed to provide an opportunity for interactive user corrections.

The program generates an input file which is formatted to be read by the simulator. The data are written to file so that the input can be saved and/or modified for future simulations.

Information about the operation of the program is included in the user manual (Carling, 1986). To simplify working with the program, the naming conventions used in DYCONDIST are also followed in the input generator.

2.5.2 Post-Processor

Column profiles and plots of the transient behaviour of the column variables provide much information in a compact form. The simulator produces an output file which lists column parameters at specified print intervals. These data are used by a post-processor plotting program to generate plots specified by the user.

The plotting program, PLOTTER, is written in Fortran 77 and utilizes the DISSPLA plotting package (ISSCO, 1981). The program is interactive and menu-driven. It is possible to generate multiple plots in a single session and to use output data files from multiple simulations. Further details and directions are included in the DYCONDIST user's manual (Carling, 1986).

2.5.3 Spline Interpolation

As noted in Section 2.2.3, the simulator permits interpolation of enthalpy and equilibrium coefficient data when these data are available as functions of temperature. This feature was written using cubic spline interpolation as described by Forsythe *et al*. (1977). As discussed in the DYCONDIST user manual, the knots (data points) must be presented in order of increasing temperature. In the case of equilibrium coefficients it is assumed that the abscissa values of the data points may be different for each component. In the case of vapour and liquid enthalpies the assumption of a single set of abscissa values is made.

The spline interpolation routines were tested using data presented by Renfroe (1965).

2.5.4 Partial Condenser Model

Although the version of the simulator used by Wong (1985) was said to have the capability of modelling partial condensers, it was found that this feature had been incorrectly implemented. For a partial condenser the generalized stage material balance (Equation 2.1) becomes:

$$\frac{dM_1}{dt} = V_2 - V_1 - L_1 - D \qquad (2.23)$$

This assumes that there are no feeds to or draws from the condenser. Two cases exist for the calculation of flow rates V_1, L_1 and D. For the case of open loop simulations, perfect level control is assumed. The case of variable liquid holdup in the accumulator drum is considered in Section 5. In either case, the calculations will depend on the specifications or control strategy assumed. To illustrate the logic, consider the case of an accumulator drum with constant molar liquid holdup when a constant reflux rate has been specified. Equation 2.30 then becomes:

$$V_2 = L_1 + V_1 + D \tag{2.24}$$

Since V_1 and (L_1+D) are in equilibrium, the tray energy balance is used to calculate the vapour distillate rate, V_1. The liquid rate (L_1+D) may then be calculated using Equation 2.31 and the fact that the liquid distillate rate, D, is the difference between the liquid from the accumulator drum and the specified reflux rate. Since the partial condenser is an equilibrium stage, the liquid and vapour compositions are determined by integration of Equation 2.2.

Other control situations must be considered separately. Common specifications are incorporated into the current version of the simulator. Others may be added as required.

2.5.5 Control Strategy Implementation

Including models for local and remote controllers alters the solution procedure outlined in Figure 2.3. For local controllers, the calculations of elements of the Jacobian in Equations 2.15 and 2.16 must be modified and the dimension of the system of equations is increased. For remote controllers the control calculation block shown in Figure 2.3 is required, adding steps to the overall computation. These issues are discussed in Chapter 4 where the development of control loop models and the resulting modifications to the simulator are discussed.

3. OPEN LOOP SIMULATION EXAMPLE

3.1 Introduction to Depropanizer Example

The primary example studied in this work is a depropanizer tower. This example is based on one presented by Cook (1980) and Ballard *et al.* (1978) and was subsequently modified by Wong (1985). The choice of a depropanizer is appropriate since it is an industrially important type of tower in that depropanizers are not only common, but such columns are typical of many other light ends towers. This chapter examines open loop simulation results for this example. Control strategy development work for the example is discussed in Chapter 5.

A schematic diagram of the column is given in Figure 3.1. The tower has 29 stages, a partial condenser and partial reboiler. There is a single saturated liquid feed consisting of ethane, propylene, propane, isobutane, and cisbutene (cis-2-butene) entering at stage 12. Component liquid and vapour enthalpies are evaluated as polynomial functions of temperature within the pressure range of the tower. A similar approach is taken for the equilibrium coefficients. Liquid enthalpies are correlated as simple first order functions of temperature:

$$h_i = a_{0i} + a_{1i}T \tag{3.1}$$

where the enthalpy is in kJ/kmol and the temperature

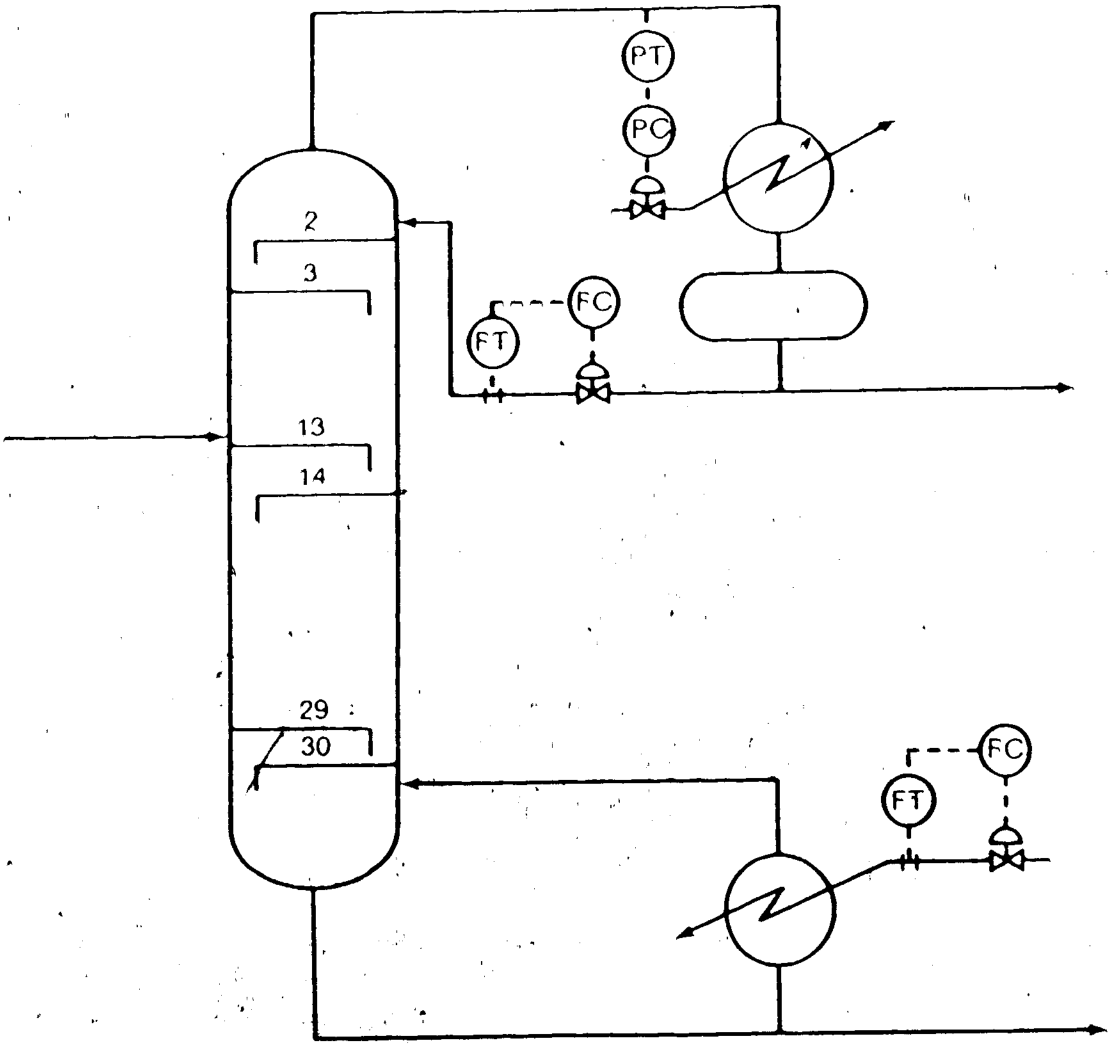


Figure 3.1

DEPROPANIZER SCHEMATIC DIAGRAM

is in K. Vapour enthalpies are expressed as second order polynomials

$$H_i = b_{0i} + b_{1i}T + b_{2i}T^2 \tag{3.2}$$

Equilibrium ratios are fitted to functions of the form

$$\ln(K_i) = c_{0i} + \frac{c_{1i}}{T} + \frac{c_{2i}}{T^2} \tag{3.3}$$

The coefficients of the polynomial functions have been tabulated by Wong (1985) and are included in this work for convenience as Appendix A.

3.2 Open Loop Results

3.2.1 Base Case Steady State Conditions

Establishment of base steady state conditions provided a benchmark against which to study column dynamic response to various disturbances. Constant molar tray liquid holdup was assumed for the base case. Accumulator and base surge holdups were also assumed to have constant molar values. A summary of column feed and operating conditions is given in Table 3.1. The temperature and composition profiles determined using the simulator are presented in Figures 3.2 and 3.3 repectively. These differ slightly from those presented by Wong (1985) because of the differences in the condenser modelling which were discussed in Section 2.5.4 and because of a correction to one coefficient in one of the

Table 3.1

BASE CASE OPERATING CONDITIONS

Feed:	
Temperature	353. K
Pressure	2.65 MPa
Composition (mole fractions)	
ethane	0.03
propylene	0.40
propane	0.15
isobutane	0.15
cisbutene	0.27
Rate	50. kmol/min
Operating Conditions:	
Pressure	2.65 MPa
Reflux Rate	90. kmol/min
Reboiler Duty	500. kJ/min
Condenser Duty	566. kJ/min
Accumulator Holdup	50. kmol
Column Base Holdup	50. kmol
Product Rates and Purities:	
Vapour Distillate Rate	3.6 kmol/min
Liquid Distillate Rate	25.0 kmol/min
Bottoms Rate	21.4 kmol/min
Heavy Key in Liquid Distillate	0.44%
Light Key in Bottoms	1.59%

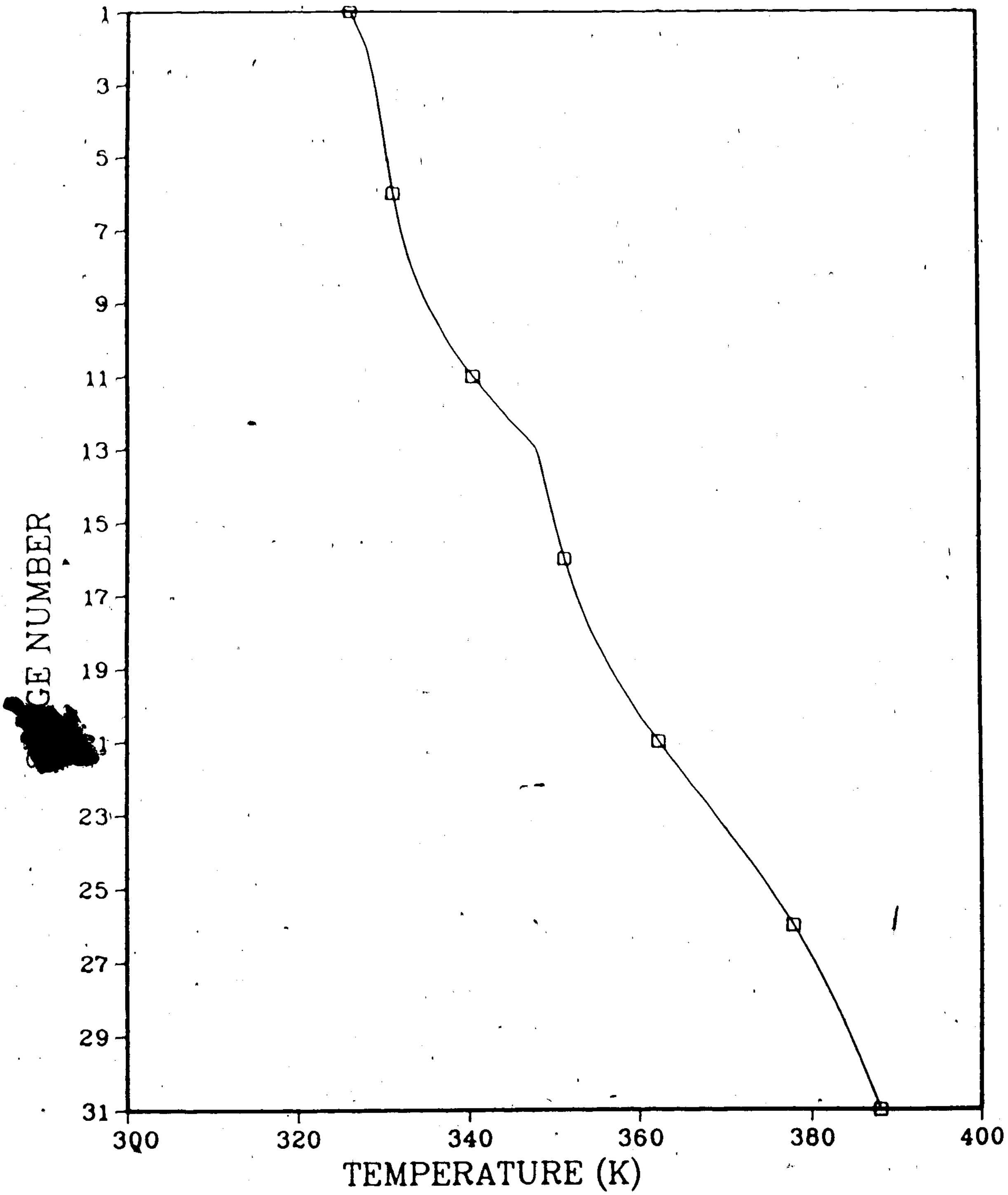


Figure 3.2

BASE CASE STEADY STATE TEMPERATURE PROFILE

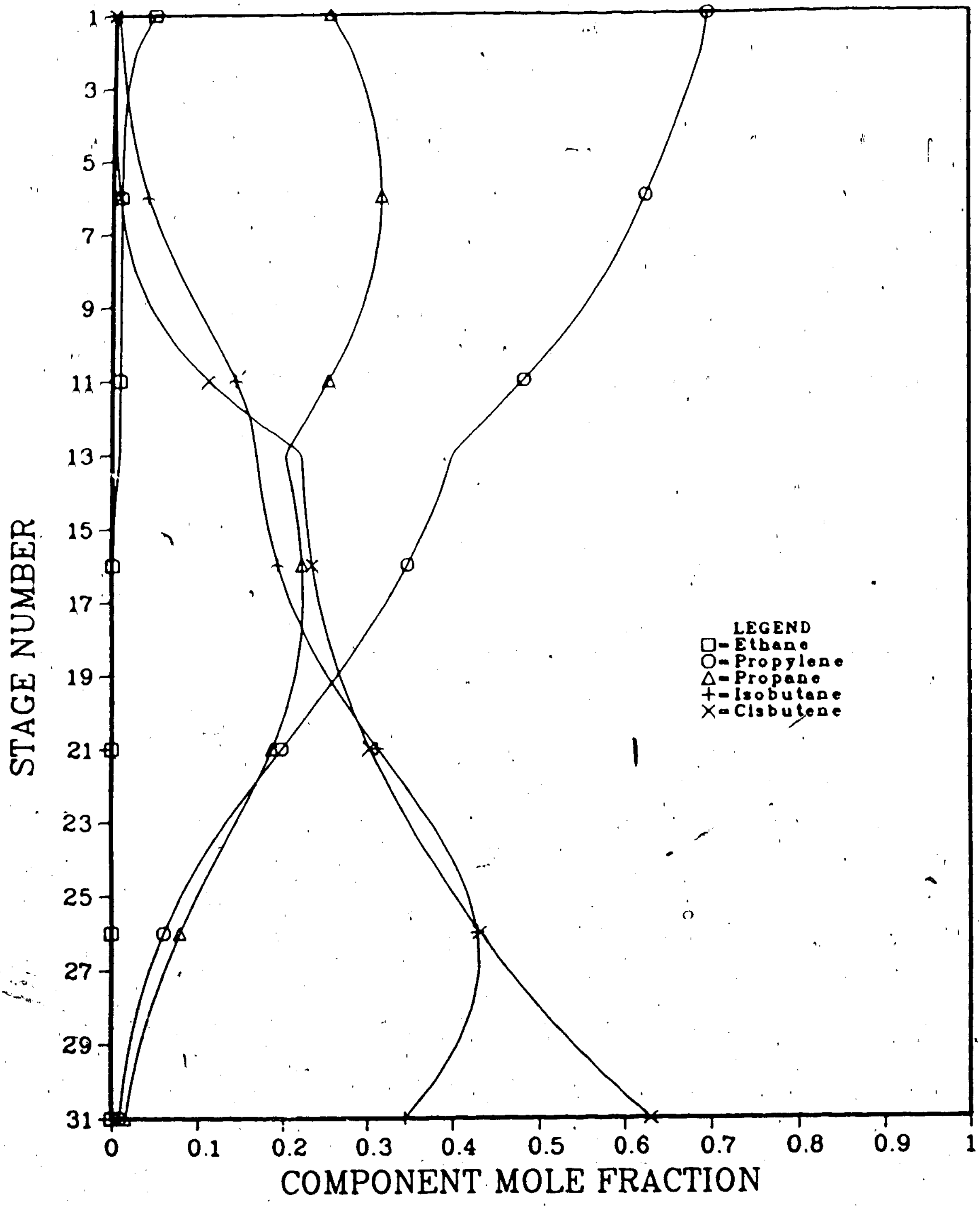


Figure 3.3

BASE CASE STEADY STATE COMPOSITION PROFILES enthalpy correlations. In previous work on simulation of the column a constant tray holdup of 14 kmol per stage was assumed (Cook, 1980; Wong, 1985). As an improvement on the assumption of the same constant holdup on each tray, the holdups were assumed in this study to be time invariant but dependent on tray location. The holdup distribution was calculated for the base operating conditions using a variable holdup option as discussed in Section 3.3.

3.2.2 Feed Rate Disturbances

The simulator was subjected to a series of step changes in feed rate. Product composition responses were studied as were temperature responses. In each case the initial conditions used corresponded to those described in the previous section. Transients of one hour were simulated and examination of the final conditions indicated that a new steady state was reached in most cases. An additional hour of operation was simulated for cases in which simulation showed that the process was not at steady state after the first hour.

Feed rate increases and decreases of ten and thirty percent were studied. The cases were run with specifications of constant reflux rate and reboiler duty. Base case values of 90 kmol/min and 500 kJ/min respectively were maintained. Feed composition and conditions were as listed in Table 3.1.

Figures 3.4 through 3.7 illustrate the product composition responses for each case. It should be noted that the ordinate values are deviations from the base case component mole fractions. An interesting feature of some of these responses is that they are nonminimum phase. For example, the mole fraction of isobutane in the bottoms product initally increases in response to a 30% increase in feed rate before it eventually decreases. As shown in Figure 3.7, the final value is less than the inital value. Table 3.2 summarizes the instances of inverse response noted for feed rate disturbances.

A simple criterion is required to identify inverse responses of column variables since it is infeasible to plot every transient response. For each composition and temperature response the initial value, first transient value and final value are compared. If the direction of the deviation between the first transient value and the initial value is not the same as that between the final value and the initial value, then the transient is deemed to exhibit inverse response behaviour. There are some limitations to this inexpensive check: the following examples demonstrate that the procedure can miss certain instances of inverse response and that it can flag a transient as displaying inverse response behaviour when none exists. If the value of a column variable initially increases in response to a disturbance before decreasing below the initial value it would be flagged by the procedure as displaying inverse

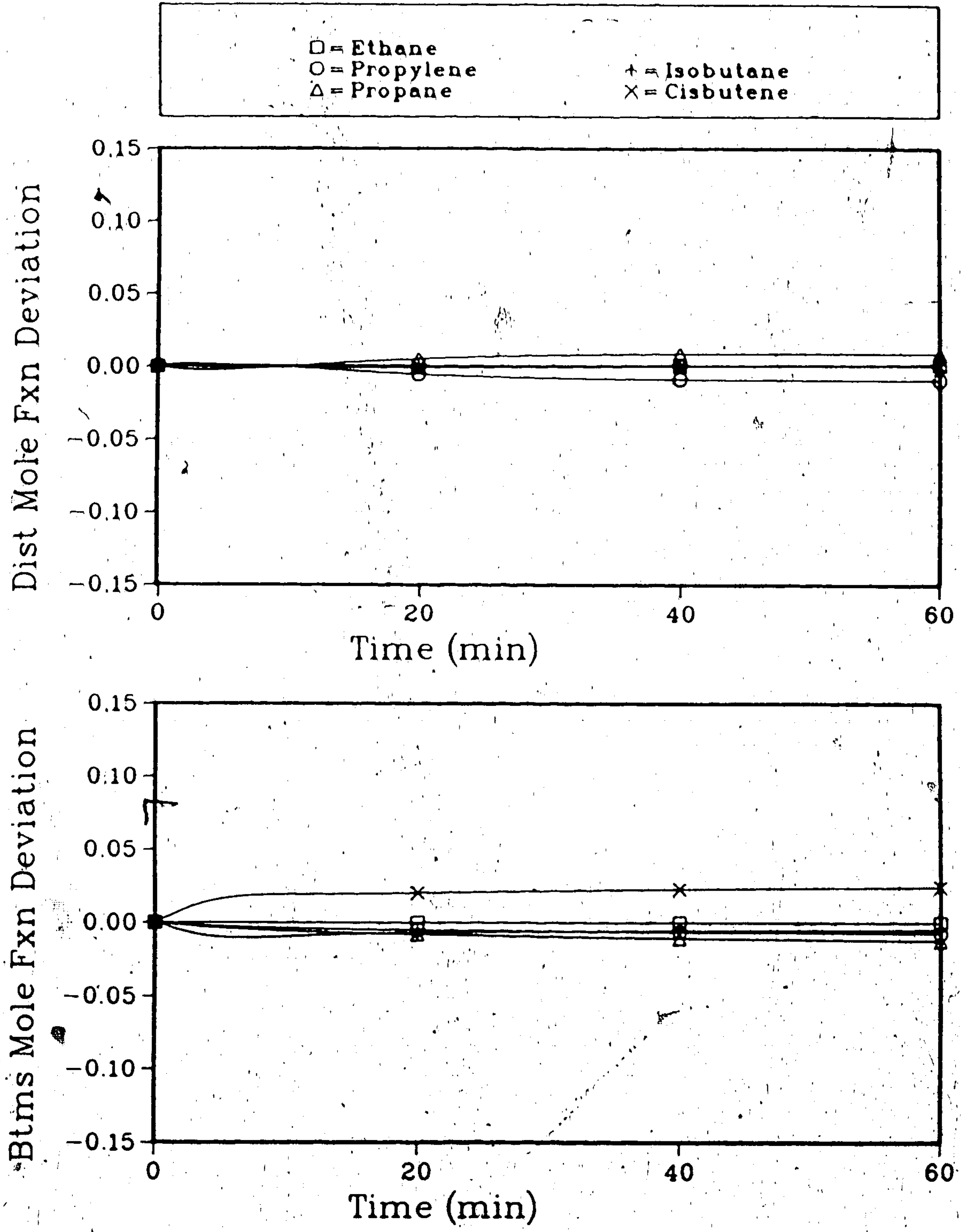


Figure 3.4

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 10% FEED RATE DECREASE

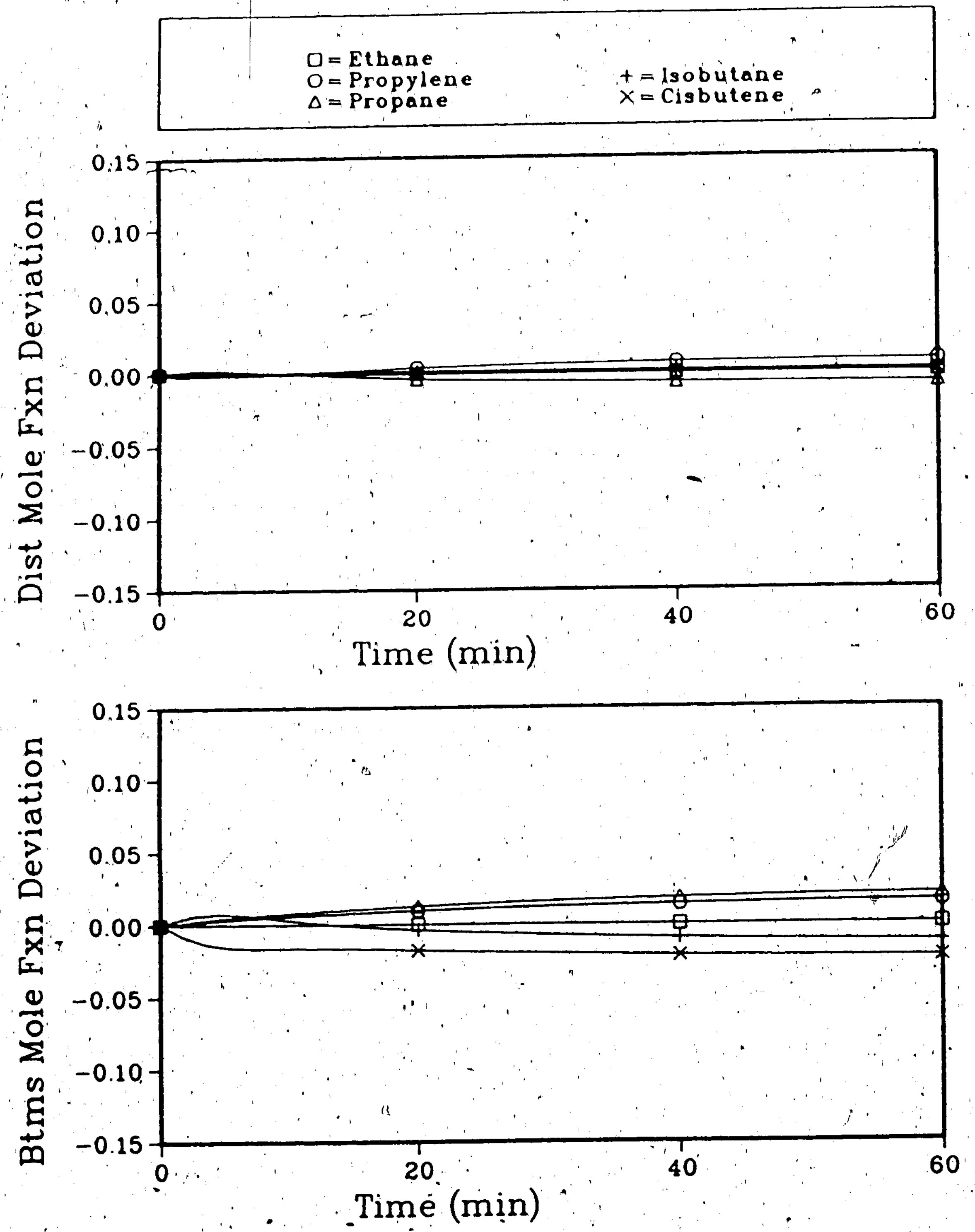


Figure 3.5

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 10% FEED RATE INCREASE

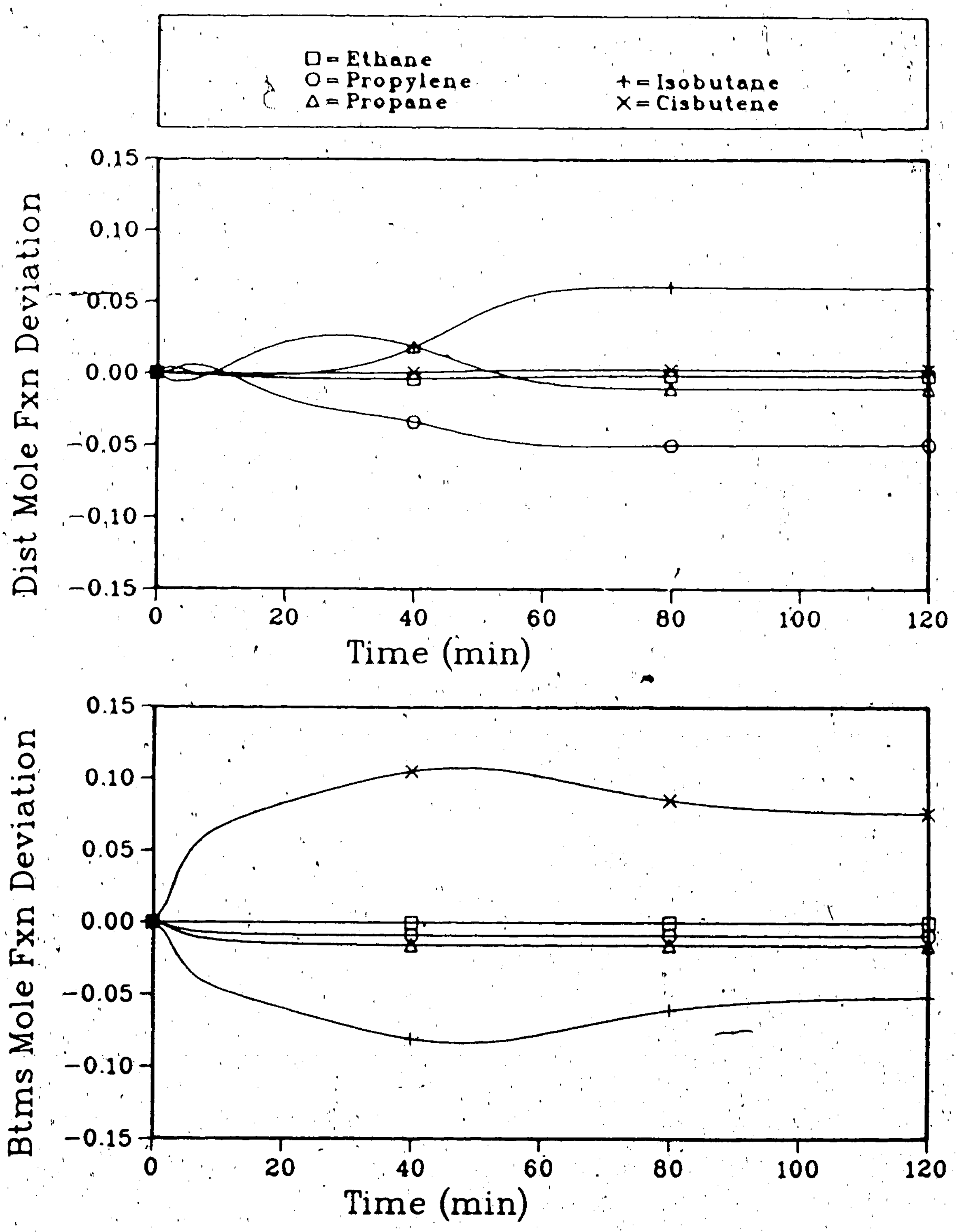


Figure 3.6

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 30% FEED RATE DECREASE

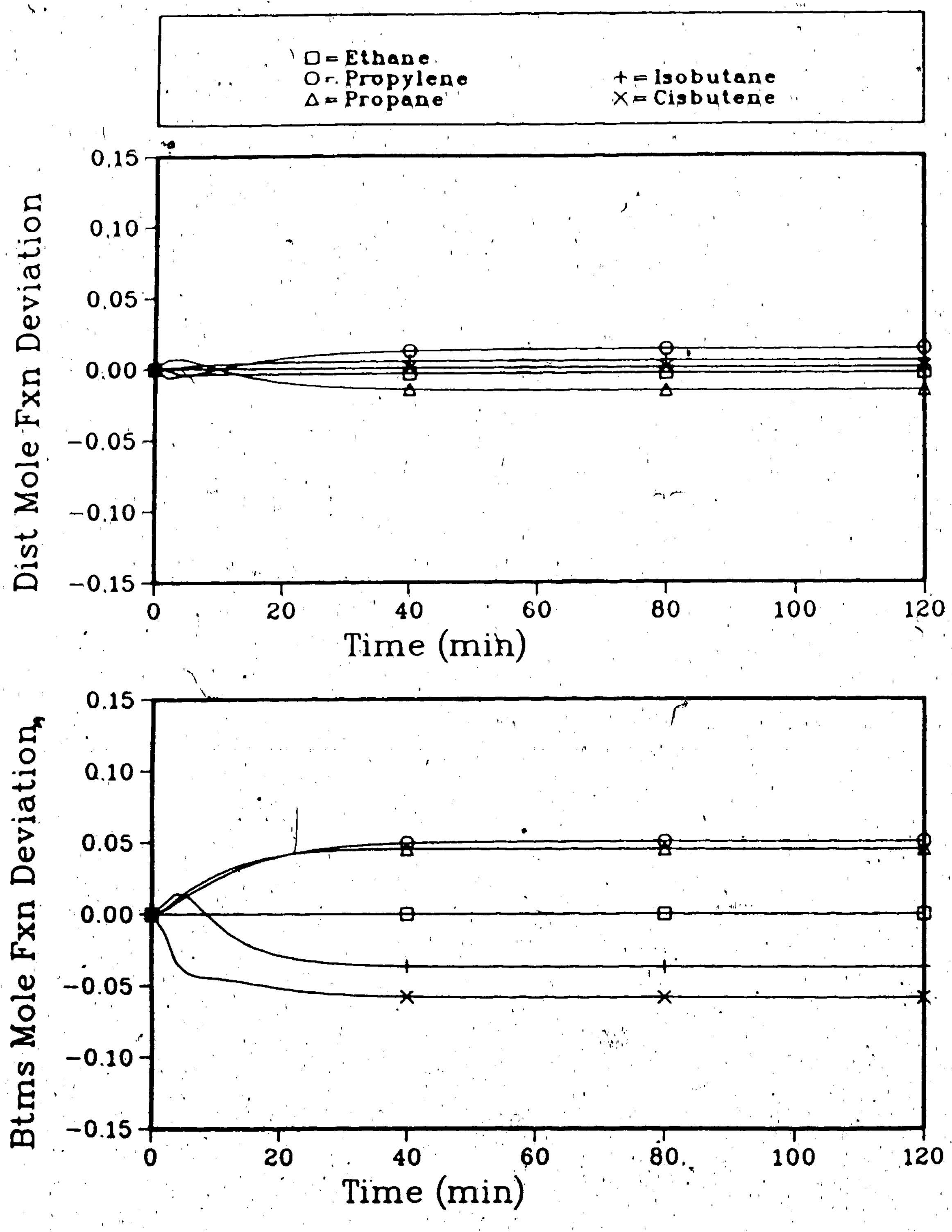


Figure 3.7

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 30% FEED RATE INCREASE

Table 3.2

SUMMARY OF INVERSE RESPONSE BEHAVIOUR FOR FEED RATE DISTURBANCE CASES

CASE	STAGES DISPLAYING INVERSE RESPONSE					
			LK	HK		
	C2	C3-	C3	iC4	cC4	Temperature
+30% feed		1'	1			
		2-4	2-4			
		14	19-20	14		
				28-30		
				31		
-30% feed	1	1'	1			1
	2					2-3
		2-14	7-17	3-12	7-17	7-17
+10% feed		1				
		2				
		3-9				
		12-13		29-30		15
				31		
-10% feed			1			
			2			
		3-13	9-17	7-11	8-16	9-15

Note:

1. Inverse response case be seen in Figures 3.6 and Figure 3.7, but is not flagged by the inverse response identification procedure since there is a time lag before the composition responds

response. If, however, its value subsequently increases such that the final value is greater than the initial value the dual inverse response would pass undetected. Dual inverse responses are unlikely to occur so that this limitation of the procedure is acceptable. On the other hand, the procedure can potentially flag changes due entirely to numerical roundoff error as being indicative of inverse response. To avoid this circumstance, a tolerance is imposed on the deviations. If a temperature deviation is less than 0.1 K then the change is neglected. If a component mole fraction changes by less than 0.001, then that change is neglected. The result is that the tables summarizing inverse responses are conservative. Very small inverse responses which might be attributed to roundoff errors are neglected. Dual inverse responses and those which do not begin at the start of the transient are not flagged.

It is difficult to state general conclusions about the nonminimum phase behaviour, but the following do appear to hold:

- there are more instances of inverse response behaviour for decreases in feed rate than for increases
- based on the product composition responses in Figures 3.4 to 3.7, inverse responses to ±30% disturbances are larger in magnitude than inverse responses to ±10% disturbances
- based on the product composition responses, inverse

responses last longer for the ±10% disturbances than for the ±30% disturbances, although steady state is reached sooner in the cases with smaller disturbances

The first two conclusions agree with what is intuitively expected. Feed rate decreases are more severe disturbances than feed rate increases, so more inverse responses might be expected. Larger magnitude disturbances lead to larger deviations from the initial steady state values than do smaller disturbances, so the same trend is expected for inverse responses. The third conclusion can be explained by consideration of the driving forces which must be smaller for small disturbances than for larger disturbances. As is the case with other examples of nonminimum phase behaviour, the inverse responses must be caused by interaction between two opposing effects. In the case of the ±10% disturbances the driving force causing the predominant effect must be smaller than for the ±30% disturbances so that it does not dominate until later in the transient.

Temperature and product composition inverse responses are of special interest since these variables are likely to serve as controlled variables for feedback control. In this respect it is fortunate that product composition inverse responses appear in the light key and lighter components in the distillate product and in the heavy key component in the bottoms.

Transient responses of column composition, temperature, and liquid flow rate profiles have been prepared to facilitate investigation of the nonminimum phase behaviour observed in response to feed rate disturbances. Figures 3.8 and 3.9 show the transient responses of the column temperature profile to a 30% feed rate decrease and a 30% feed rate increase respectively. As may be confirmed by cross-referencing Table 3.2, the +30% feed rate disturbance does not result in nonminimum phase temperature response behaviour, but the -30% feed disturbance results in inverse response of the temperatures on the top three stages (stages 1 to 3) and on the stages around the feed point (stages 7 to 17). The individual stage temperatures are seen to respond gradually to the disturbances and do not display any sudden discontinuities which might indicate numerical problems. Those stage temperatures not displaying inverse response reach final steady state values earlier in the transient than do those stage temperatures displaying inverse response.

Mole fraction responses of the key components, propane and isobutane, to a 30% feed rate decrease are shown in Figures 3.10 and 3.11. The profiles are seen to change quite dramatically over the course of the transient period. In Figure 3.10 inverse response behaviour is seen in both the rectification and stripping sections. It should be noted that the stage numbers are numbered in reverse order to the previous plots to show the rectification section

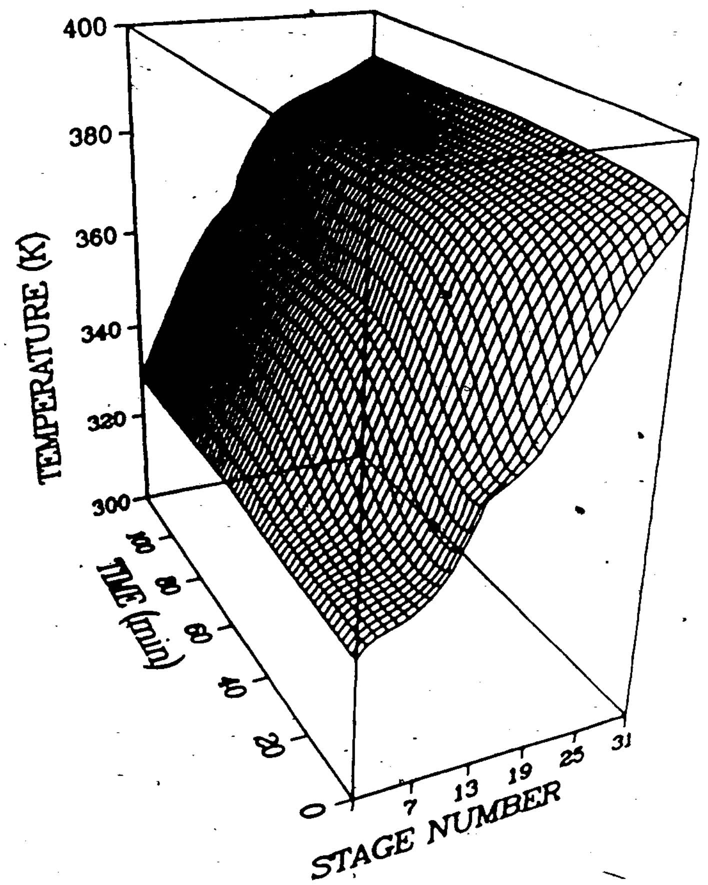


Figure 3.8
TRANSIENT RESPONSE OF COLUMN TEMPERATURES TO A 30% FEED RATE DECREASE

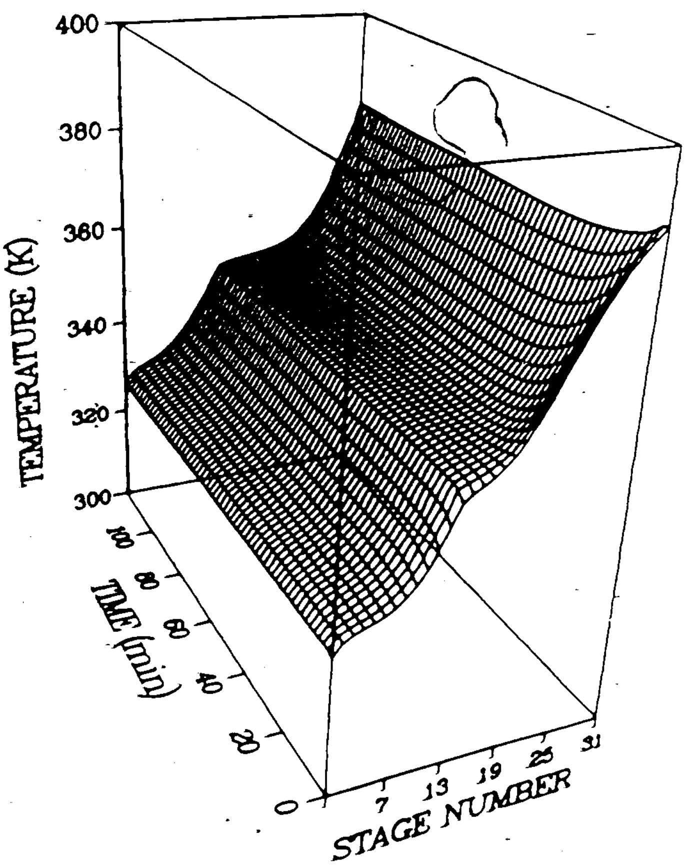


Figure 3.9
TRANSIENT RESPONSE OF COLUMN TEMPERATURES TO A 30% FEED RATE INCREASE

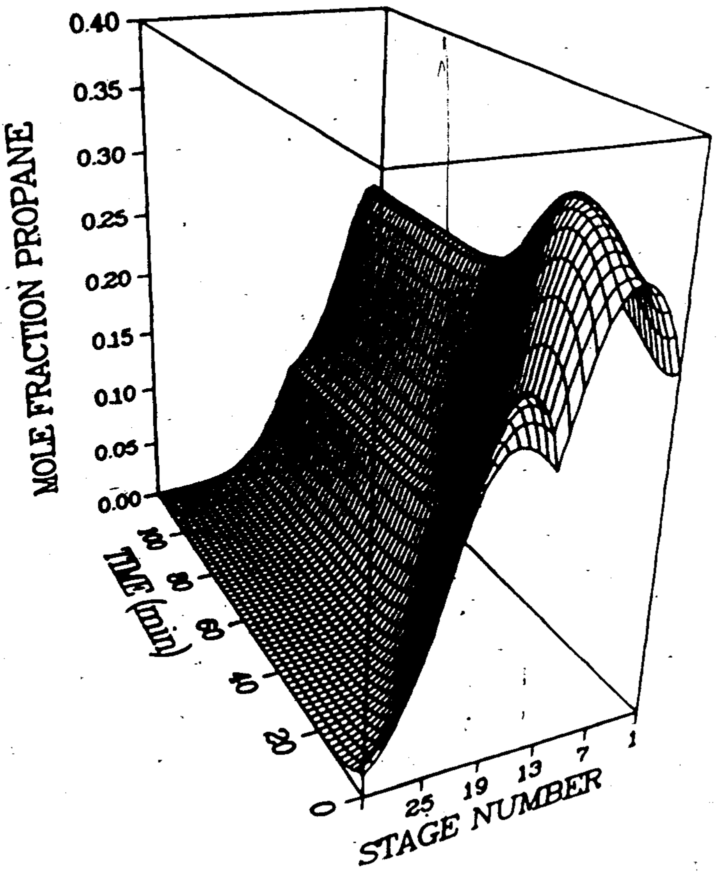


Figure 3.10
TRANSIENT RESPONSE OF PROPANE COMPOSITION PROFILE TO A 30% FEED RATE DECREASE

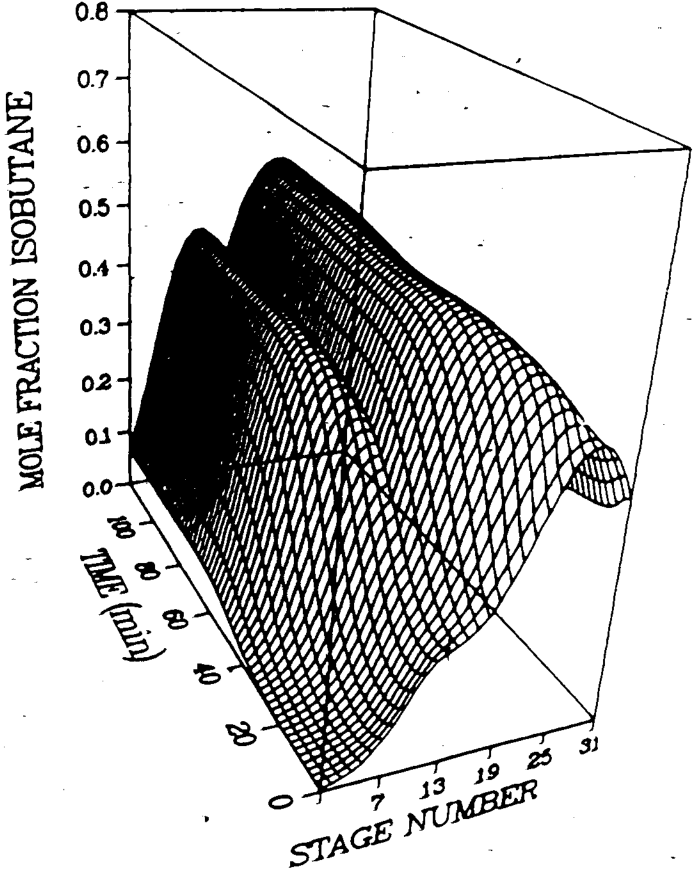


Figure 3.11
TRANSIENT RESPONSE OF ISOBUTANE COMPOSITION PROFILE TO A 30% FEED RATE DECREASE

responses more clearly. The feed tray, stage 13, can be clearly seen in the initial profile. Above the feed point (stages 7 to 12 as shown in Table 3.2) the inverse response behaviour is seen to last longer than it does below the feed (stages 14 to 17). The isobutane composition profile in the final portion of the transient shown in Figure 3.11 is bimodal with an extremum on both sides of the feed point. Inverse response behaviour is seen throughout the rectification section (stages 2 to 12) as listed in Table 3.2). In the stripping section the component mole fraction increases for all stages seen in the figure.

The mole fraction responses may be compared with the responses of the key component flow rates leaving each stage in the liquid phase. The latter responses are shown in Figures 3.12 and 3.13 and inverse behaviour is seen to occur in the same locations as in the corresponding mole fraction responses (Figures 3.10 and 3.11). In addition, the component flow rate profiles show that the initial responses in the stripping section are much faster than those in the rectification section. This is largely governed by the response of the total liquid flow rates. The speed with which the final column hydraulic profile is achieved is illustrated in Figure 3.14 in which the transient responses of stage liquid flow rates are illustrated. The initial response to the disturbance is seen most clearly in the stripping section where liquid rates instantaneously decrease. Changes in the rectification section liquid rates

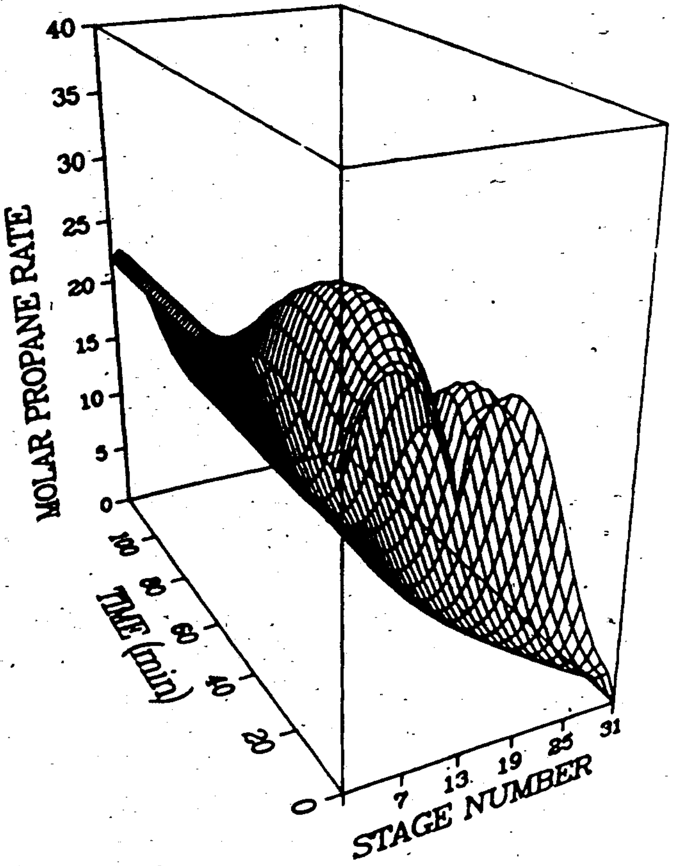


Figure 3.12
TRANSIENT RESPONSE OF PROPANE FLOW RATES TO A 30% FEED RATE DECREASE

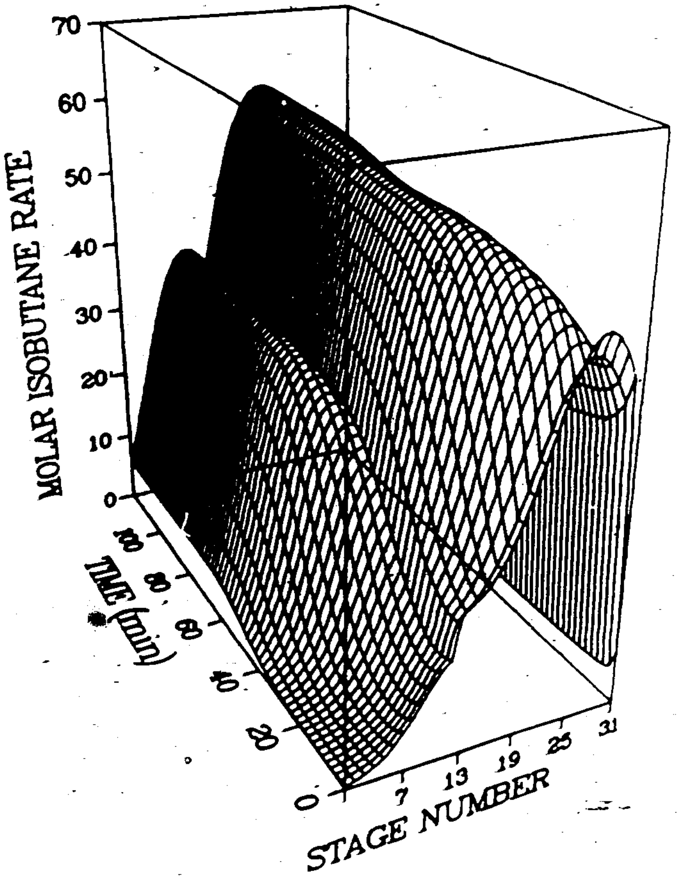


Figure 3.13
TRANSIENT RESPONSE OF ISOBUTANE FLOW RATES TO A 30% FEED RATE DECREASE

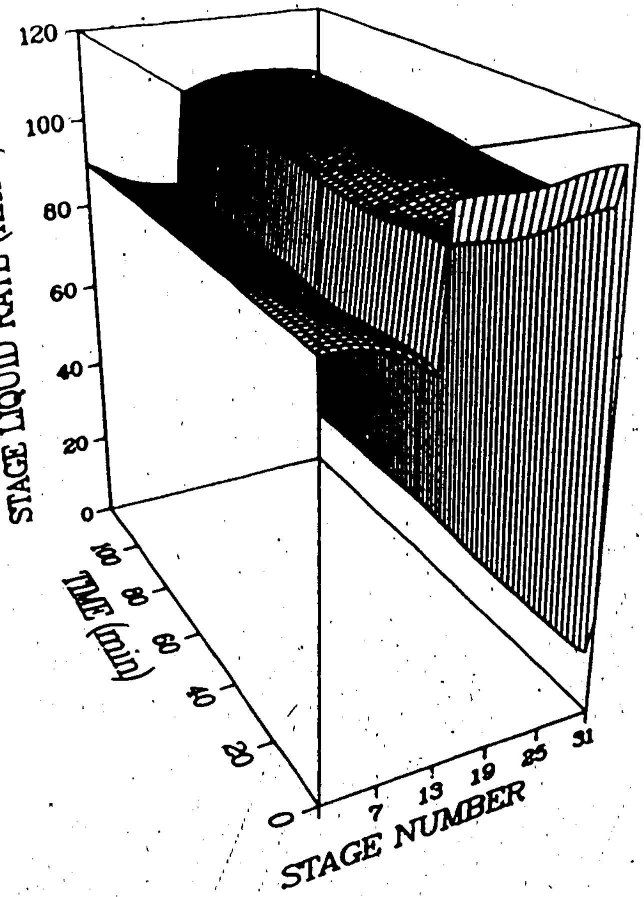


Figure 3.14

TRANSIENT RESPONSE OF COLUMN LIQUID FLOW RATES TO A 30% FEED RATE DECREASE are more gradual since the reflux rate is constant throughout the transient.

Mole fraction responses of propane and isobutane to a 30% feed rate increase are shown in Figures 3.15 and 3.16. Comparison with Figures 3.10 and 3.11 emphasizes the fact that the feed rate decrease is a more severe disturbance than the feed rate increase.

Figure 3.17 summarizes the final temperature profiles after one hour. The smaller magnitude feed disturbances, ±10%, primarily affect the stripping section temperature profile. The larger magnitude disturbances, ±30% feed rate, affect the overall profile more profoundly. The rectification section temperatures for the 30% feed rate increase case are higher than those for the base case. The crossover of the profiles as well as the lack of symmetry about the base case profile for increases and decreases of the same magnitude are further evidence of the nonlinearity of the system.

3.2.3 Reflux Rate Disturbances

Using initial steady state conditions identical to those summarized in Table 3.1, responses to reflux rate increases and decreases of 10 and 30 percent were studied. In all cases a feed rate of 50 kmol/min and a reboiler duty of 500 kJ/min were maintained.

Figures 3.18 through 3.21 show product composition responses for each case. The responses are again displayed

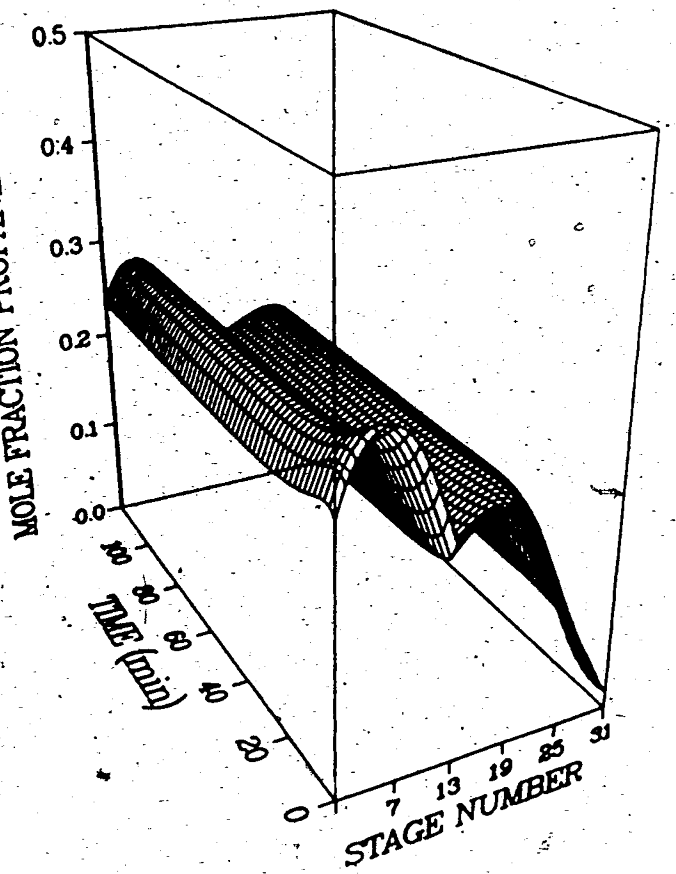


Figure 3.15
TRANSIENT RESPONSE OF PROPANE
COMPOSITION PROFILE TO A
30% FEED RATE DECREASE

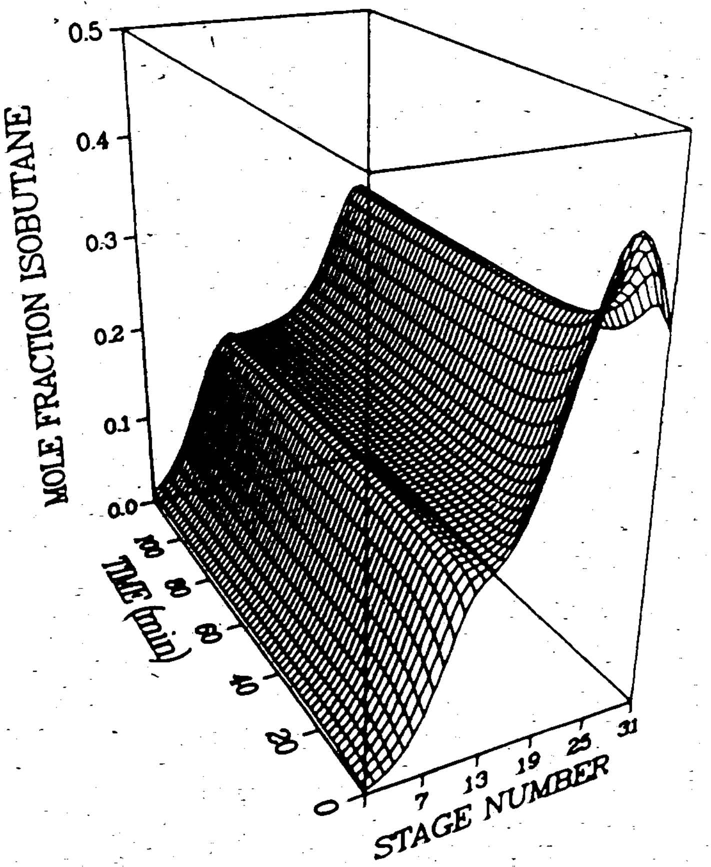


Figure 3.16
TRANSIENT RESPONSE OF
ISOBUTANE COMPOSITION PROFILE
TO A 30% FEED RATE DECREASE

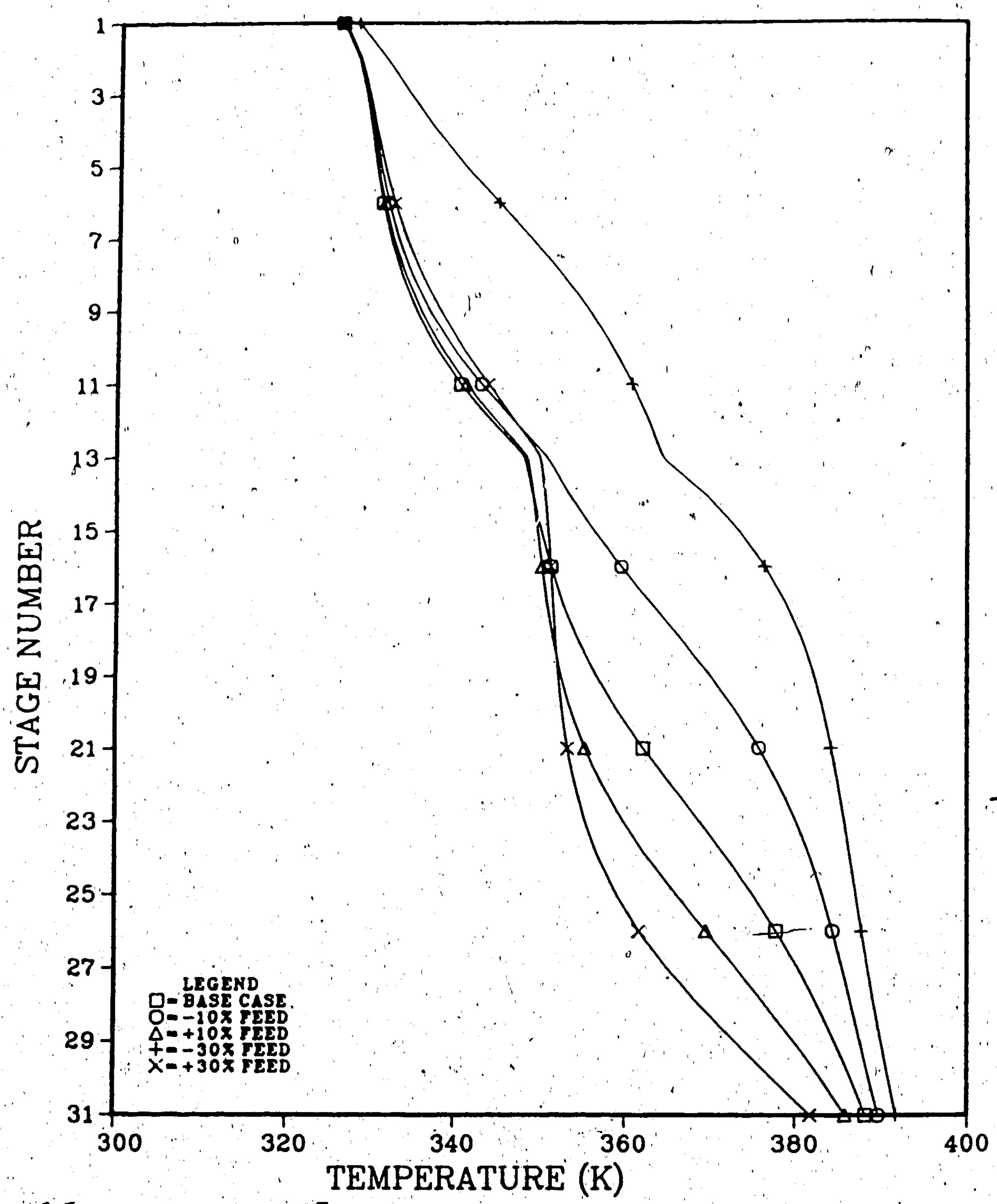


Figure 3.17

STEADY STATE TEMPERATURE PROFILES FOR FEED DISTURBANCE CASES

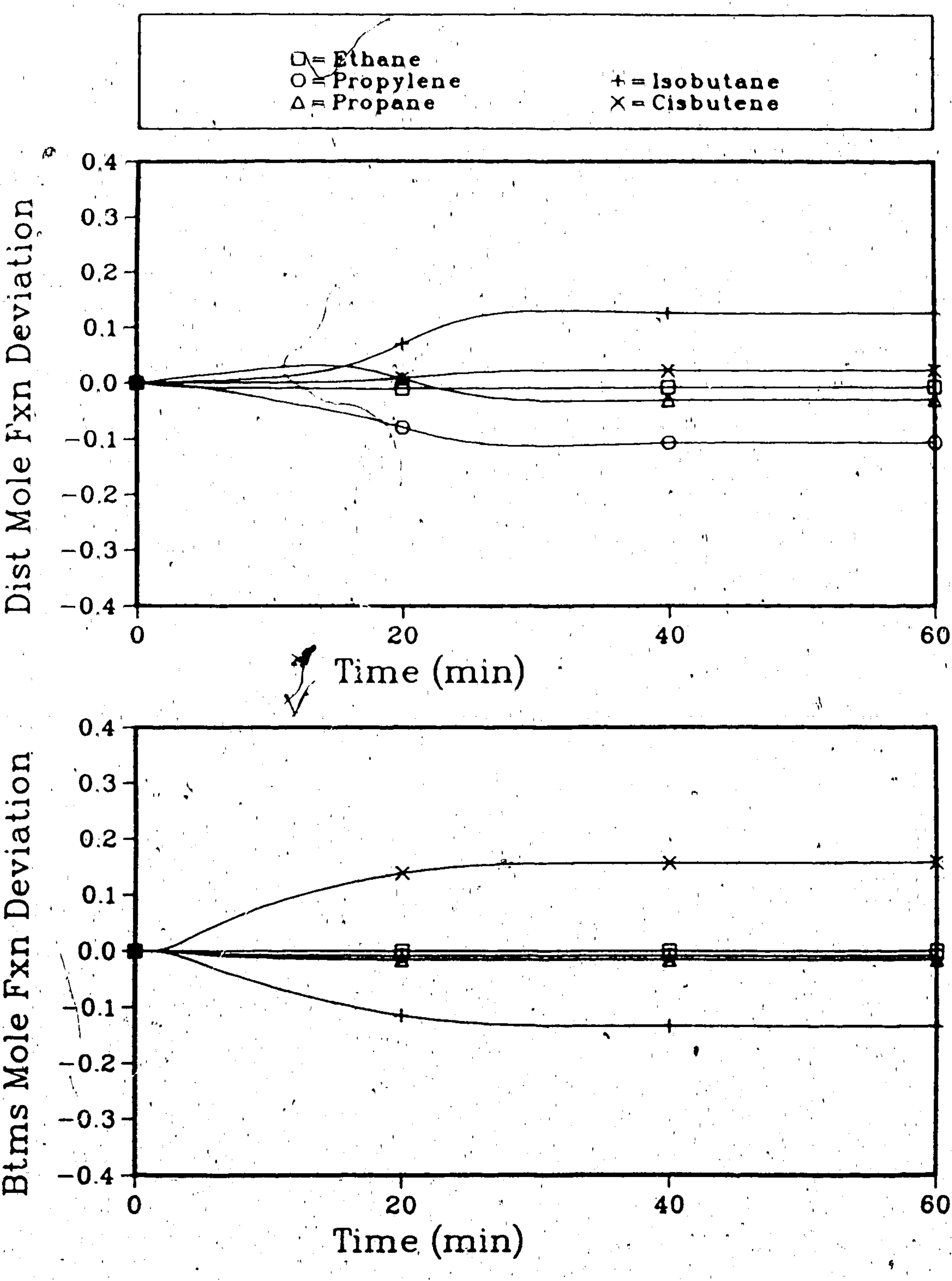


Figure 3.18

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 10% REFLUX RATE DECREASE

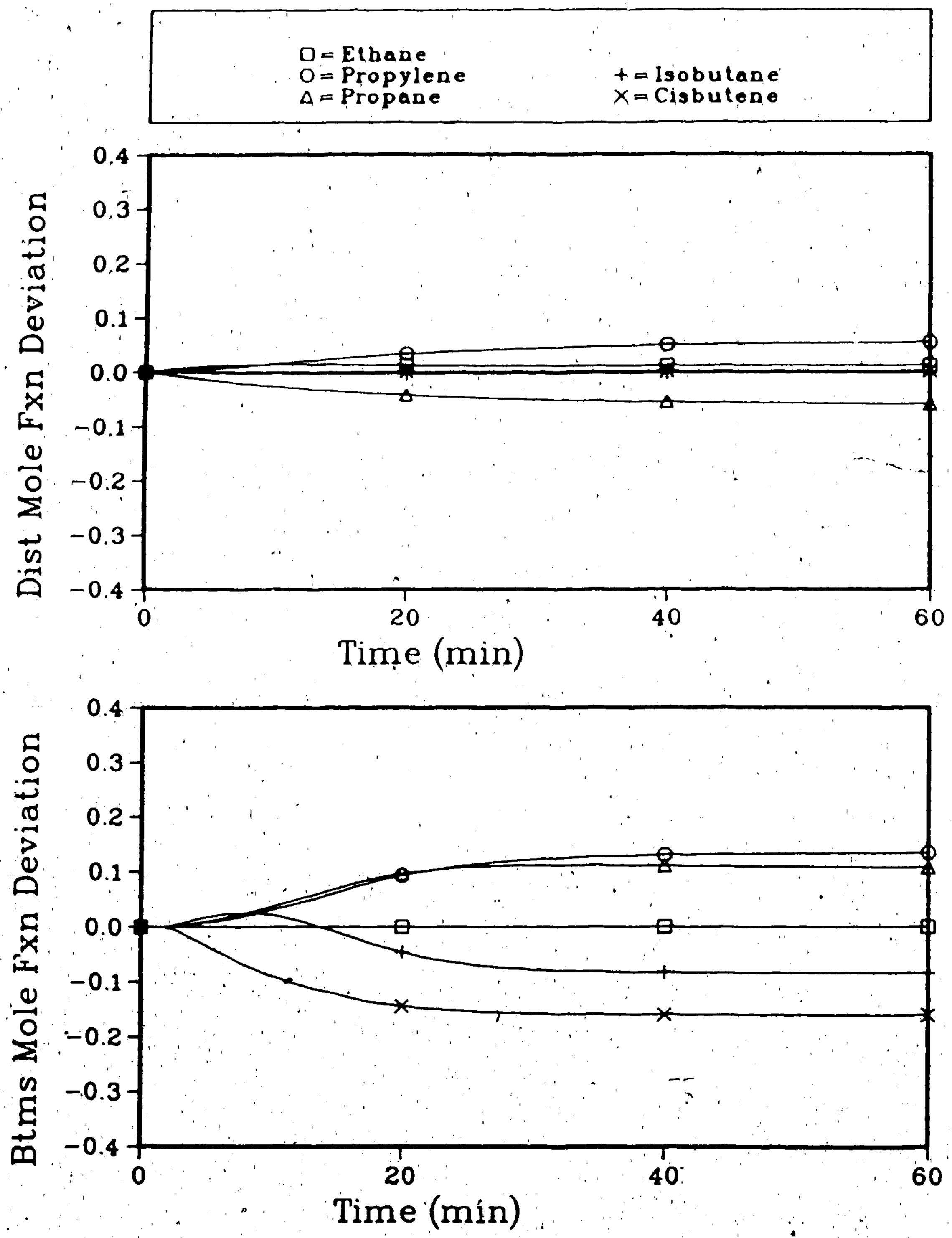


Figure 3.19

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 10% REFLUX RATE INCREASE

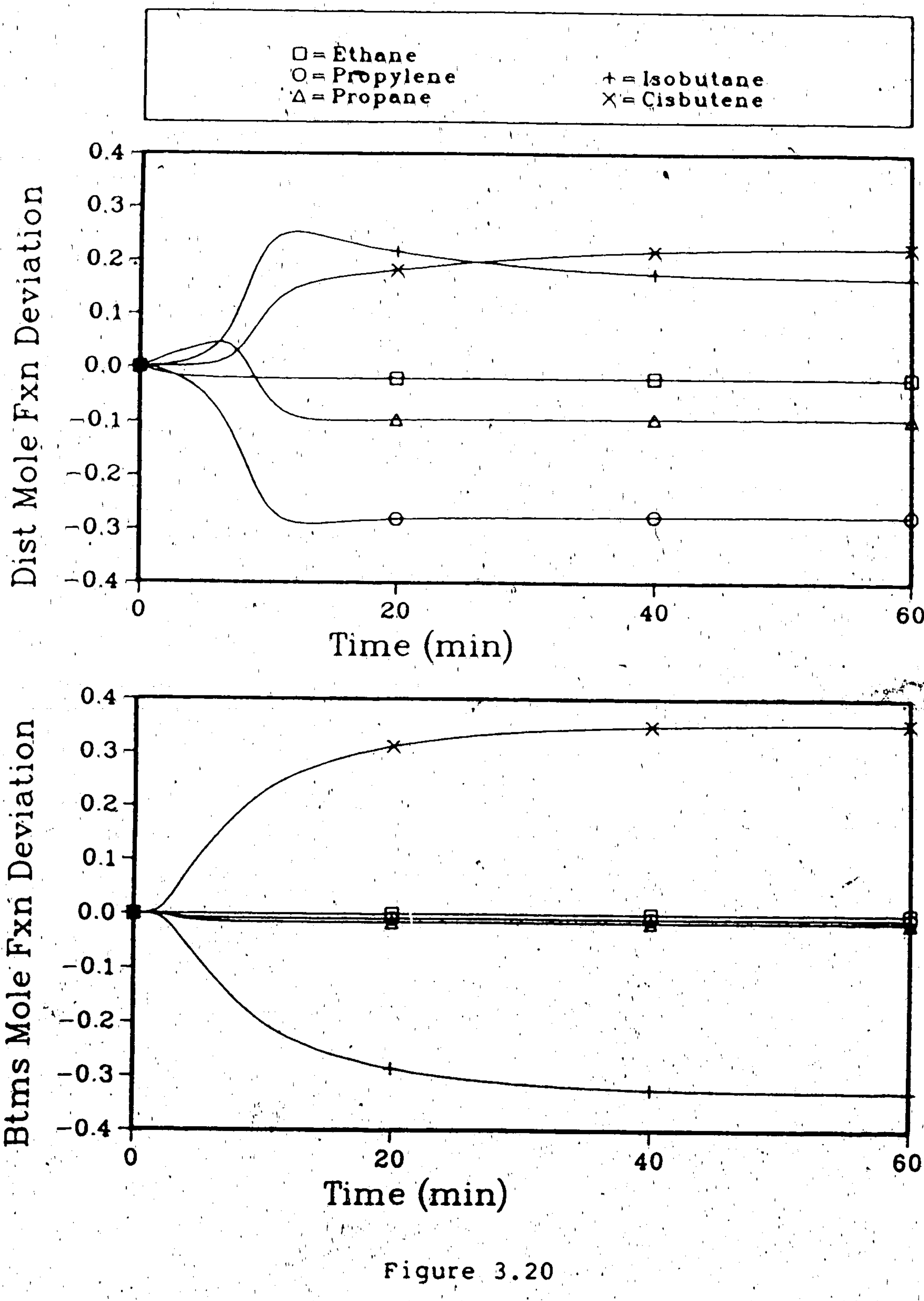


Figure 3.20

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 30% REFLUX RATE DECREASE

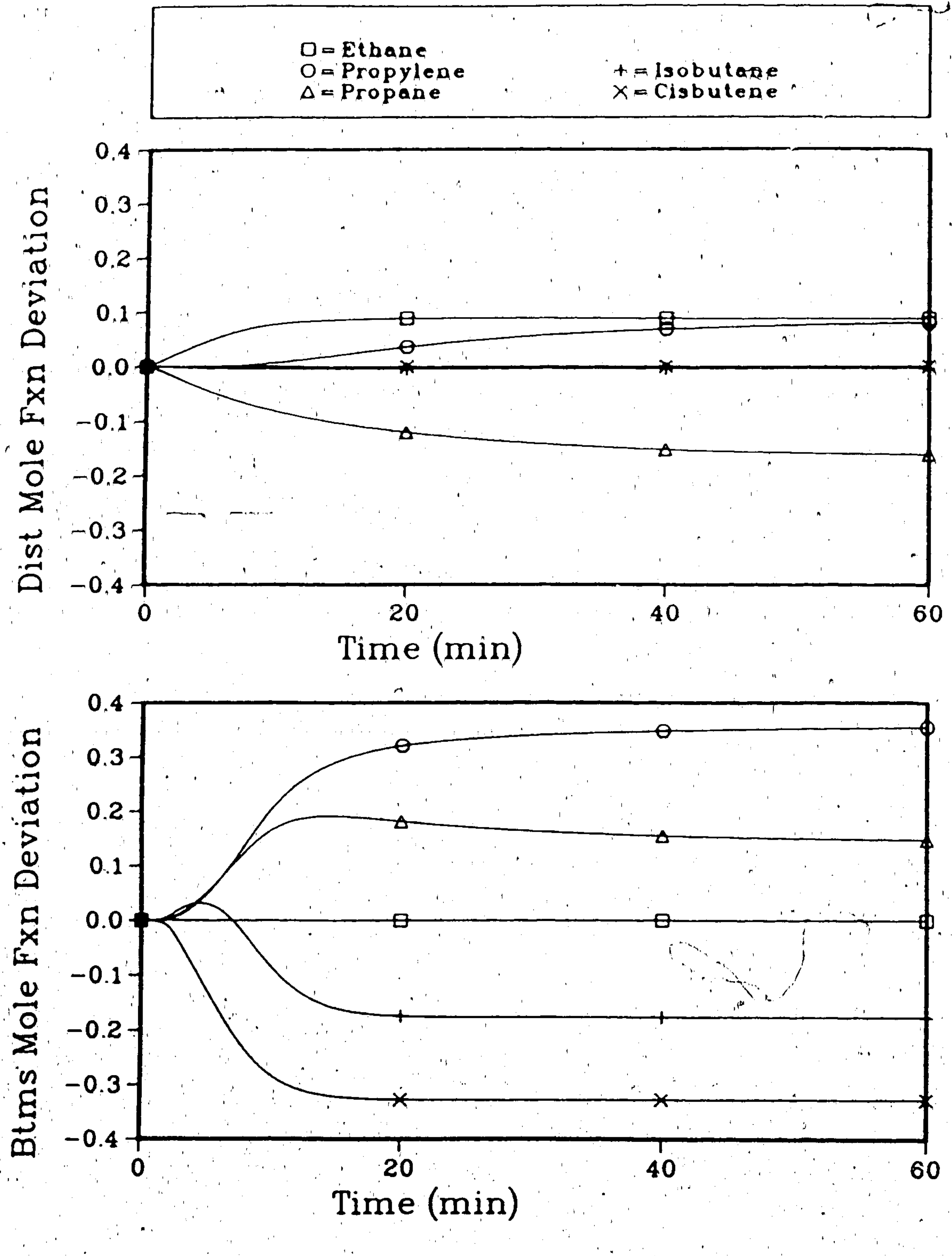


Figure 3.21

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A

30% REFLUX RATE INCREASE

as mole fraction deviations from the initial steady state values. Some nonminimum phase responses may be noted in these transients. Table 3.3 summarizes the number of column compositions and temperatures displaying inverse response.

The same procedure was used to generate the data in the table as was used in the feed disturbance cases. Tolerances of 0.1 K and 0.001 mole fraction were applied to changes in temperature and composition as was discussed in Section 3.2.2.

Inverse responses are observed in the key component compositions only. For increases in reflux rate the heavy key in the bottoms displays inverse response behaviour. For decreases in reflux rate the light key in the distillate displays similar behaviour. As was the case for feed disturbances, the fact that impurities in product streams display no inverse response implies that the behaviour will not adversely affect direct quality control. In general, the inverse responses to ±10% reflux rate disturbances are smaller in magnitude but last longer than inverse responses to ±30% reflux rate disturbances.

Figure 3.22 summarizes the final steady state temperature profiles for the reflux disturbance cases. There is nonlinearity in the response as is evidenced by the lack of symmetry about the base case profile. In general reflux rate decreases have more effect on stage temperatures above the feed point whereas reflux rate increases have more effect on temperatures below the feed point. This may lend

Table 3.3

SUMMARY OF INVERSE RESPONSE BEHAVIOUR FOR REFLUX RATE DISTURBANCE CASES

CASE	STAGES DISPLAYING INVERSE RESPONSE					
			LK	HK		
	C2	C3=	C3	iC4	cC4	Temperature
+30% reflux			8-14	31[1]		
-30% reflux			1-5	16-23		
+10% reflux				31[1]		
-10% reflux			1-5			

Note:

[1] Inverse response case be seen in Figures 3.18 and Figure 3.21, but is not flagged by the inverse response identification procedure since there is a time lag before the composition responds

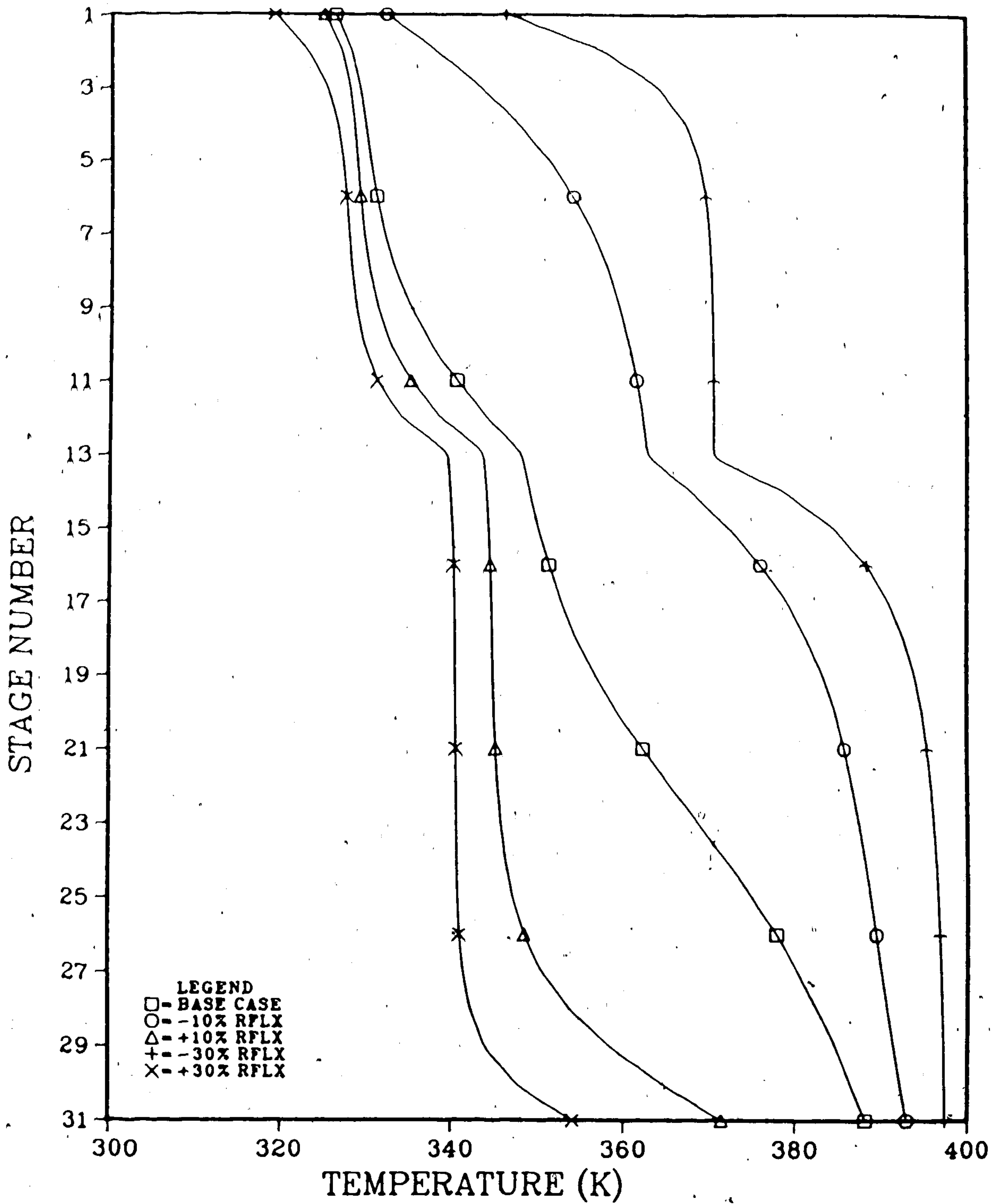


Figure 3.22

STEADY STATE TEMPERATURE PROFILES FOR REFLUX DISTURBANCE CASES support to the observation that the heavy key in the bottoms product displays inverse response to reflux rate increases whereas the light key in the liquid distillate product displays inverse response to decreases in reflux. The reflux flow rate disturbances affect the entire temperature profile, whereas for changes in feed rate the main effect was only on the stripping section temperature profile.

3.2.4 Heat Input Disturbances

Responses to disturbances in column heat input were studied by simulating transients forced by increases and decreases in reboiler heat duty. Changes of ±10% and ±30% were investigated. Initial steady state conditions corresponded to those in Table 3.1. A feed rate of 50 kmol/min and reflux rate of 90 kmol/min were specified.

Product composition transients are shown in Figures 3.23 through 3.26. Nonminimum phase behaviour was again detected with occurrences as summarized in Table 3.4.

Increases in reboiler duty lead to inverse response of the light key, propane, in the distillate. Decreases, on the other hand, lead to inverse response of the heavy key, isobutane, in the bottoms product. Inverse responses to ±10% heat input disturbances are smaller in magnitude and longer in duration than are inverse responses to ±30% heat input changes.

Figure 3.27 shows the final temperature profiles for the heat input disturbance cases. The responses are

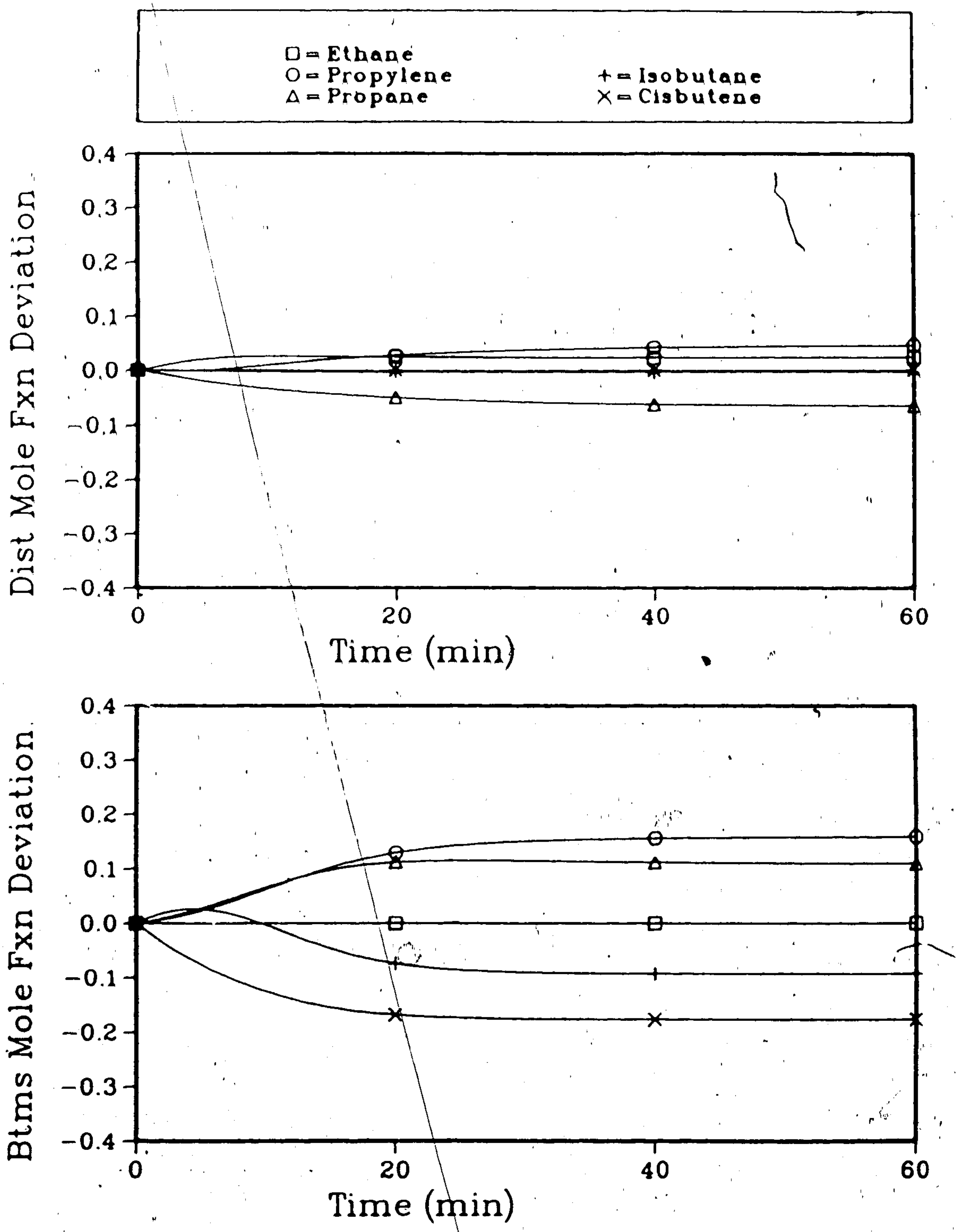


Figure 3.23

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A

10% HEAT INPUT DECREASE

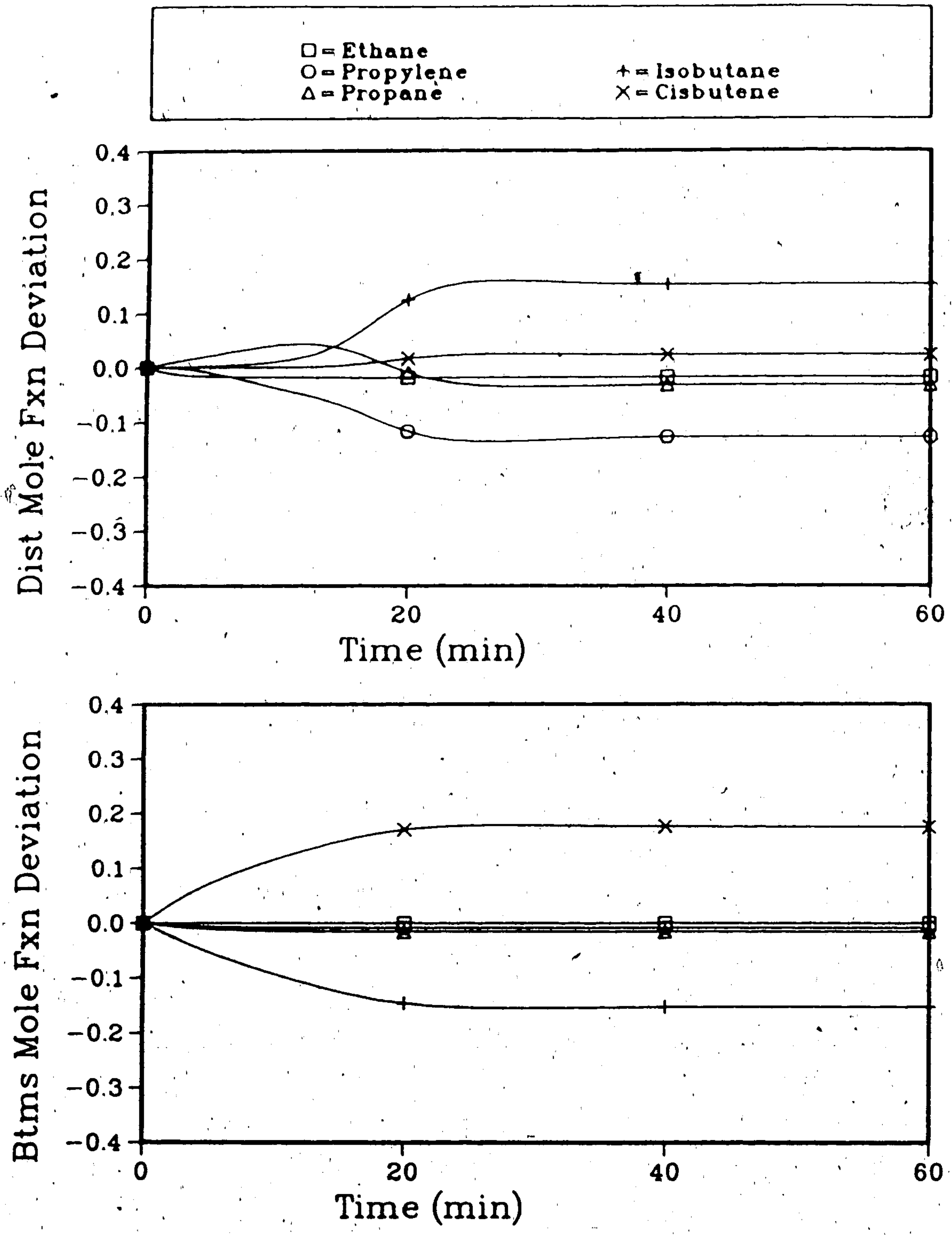


Figure 3.24

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 10% HEAT INPUT INCREASE

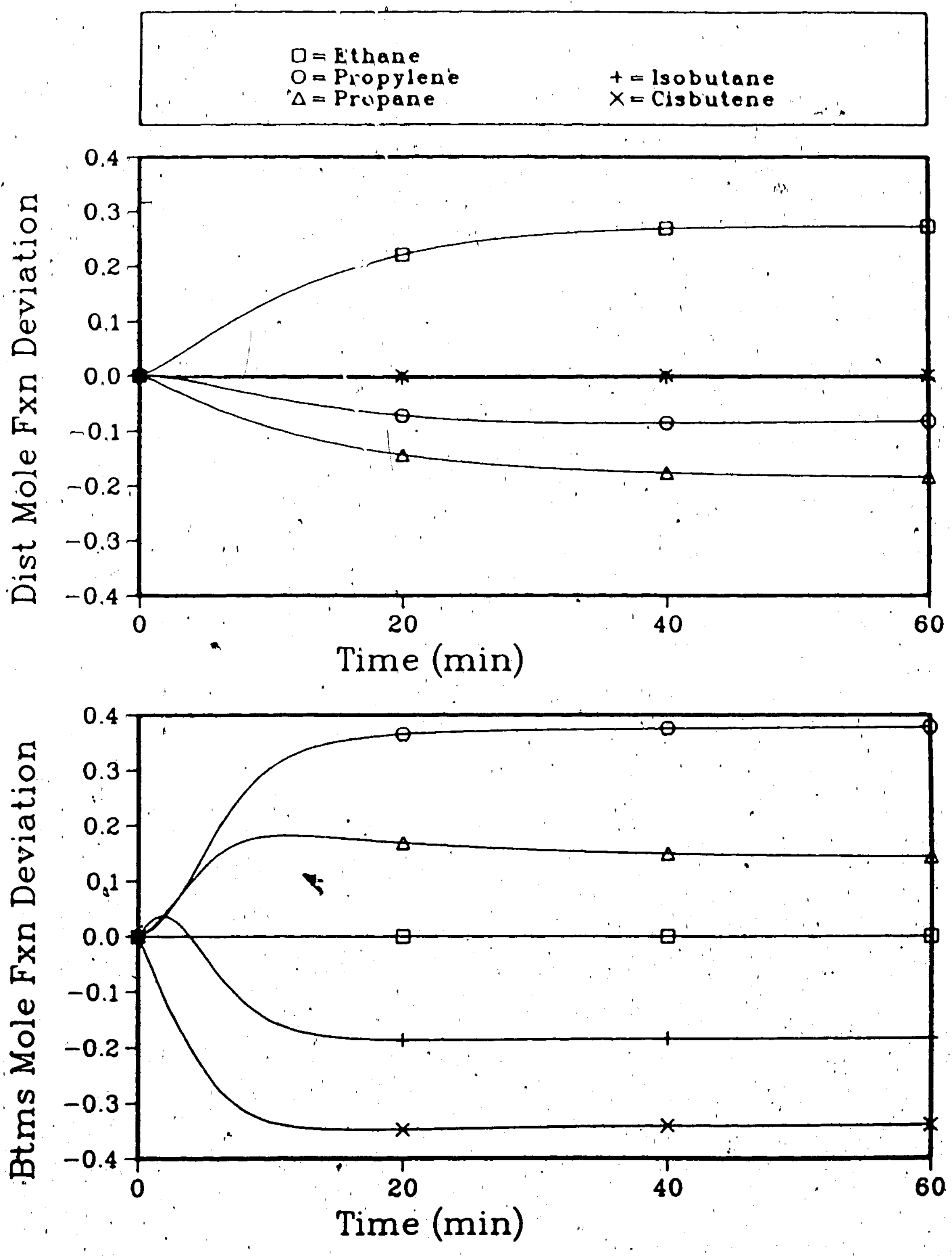


Figure 3.25

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A

30% HEAT INPUT DECREASE

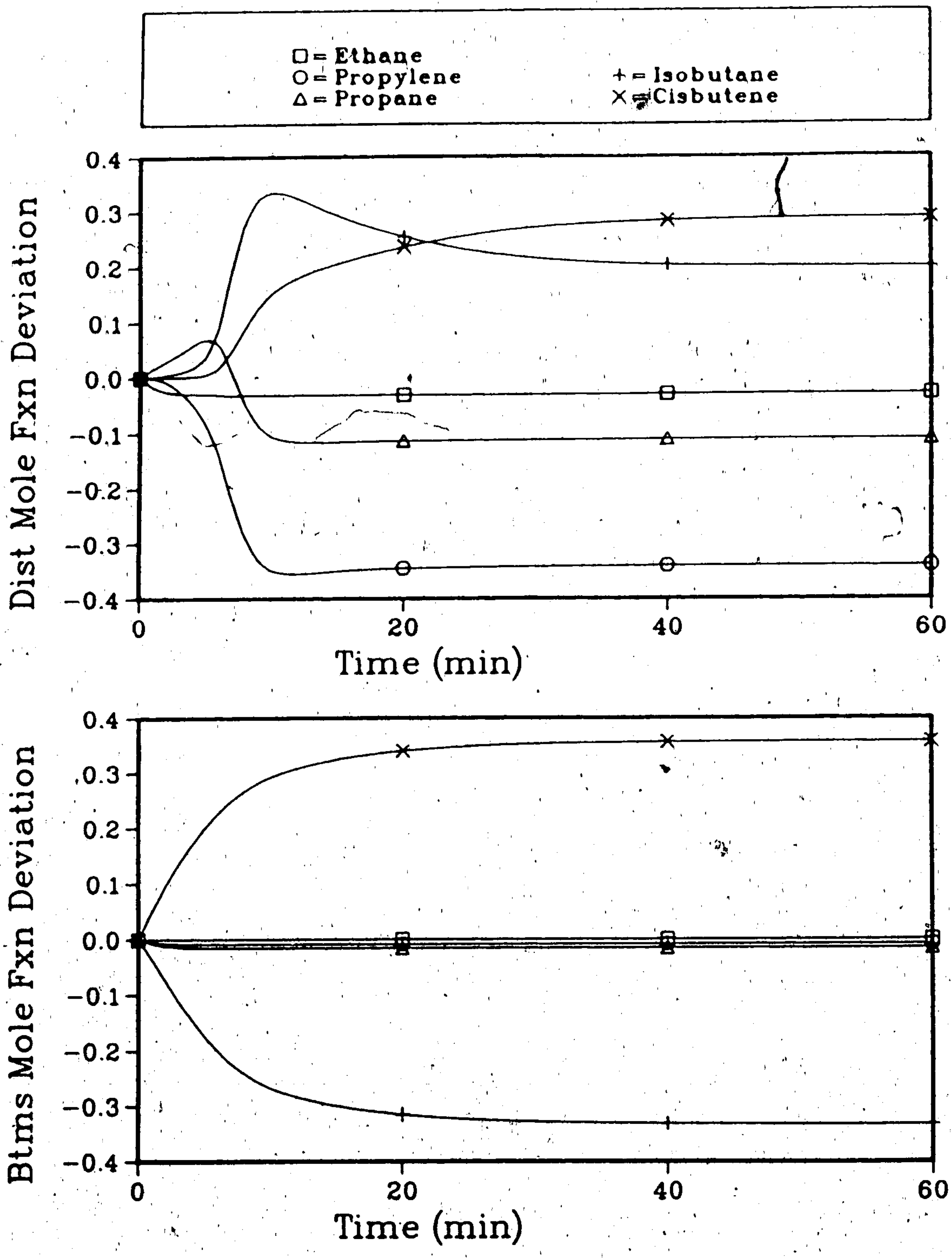


Figure 3.26

LIQUID DISTILLATE AND BOTTOMS COMPOSITION RESPONSE TO A 30% HEAT INPUT INCREASE

Table 3.4

SUMMARY OF INVERSE RESPONSE BEHAVIOUR FOR HEAT INPUT DISTURBANCE CASES

CASE	STAGES DISPLAYING INVERSE RESPONSE					
	C2	C3-	LK C3	HK iC4	cC4	Temperature
+30% QR			1-6			
			13-15	15-26		
-30% QR			8-13			
			18-21	29-31		
+10% QR			1-5			
			14-15	24-26		
-10% QR			8-12			
			18-19	28-31		

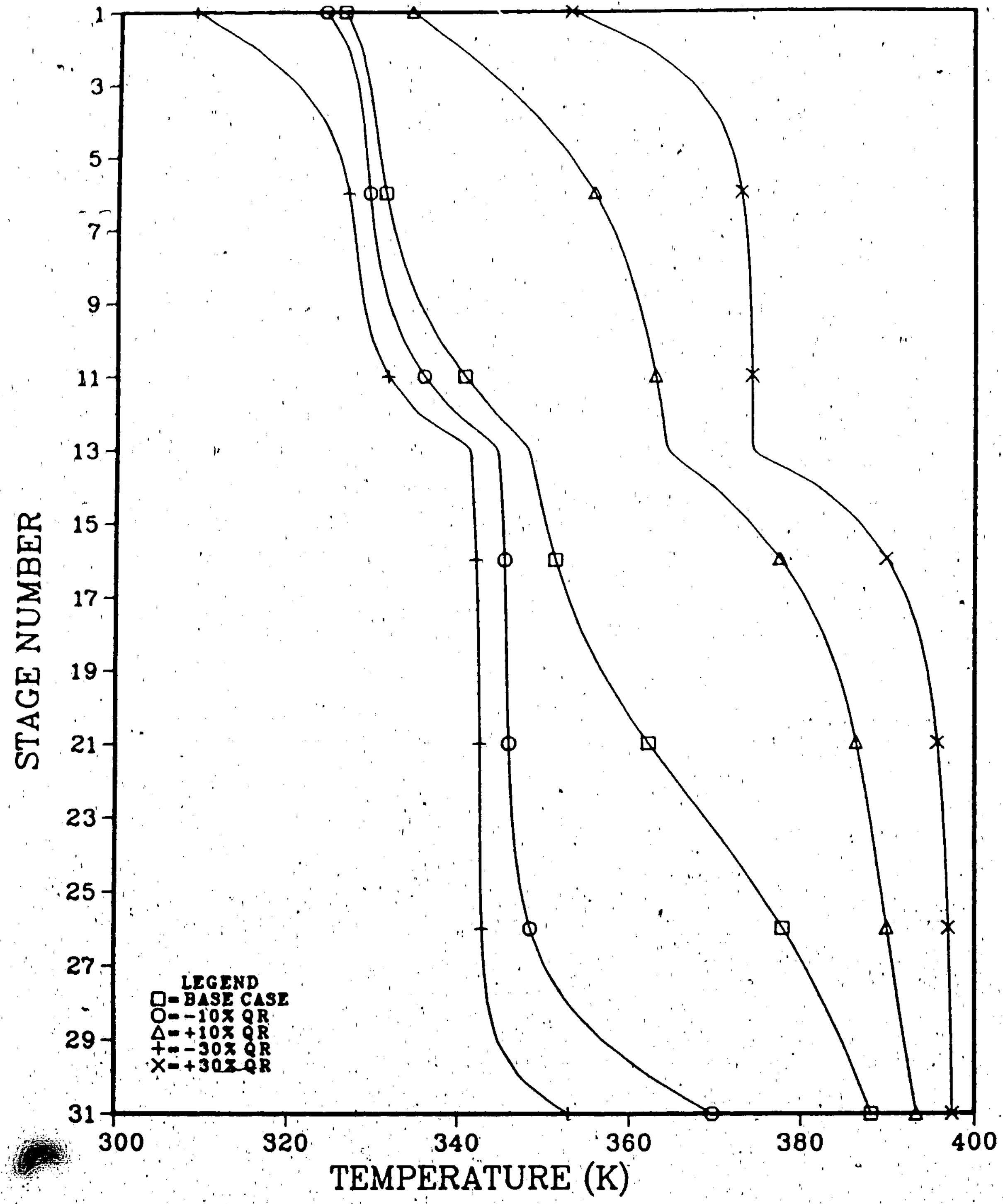


Figure 3.27

STEADY STATE TEMPERATURE PROFILES FOR HEAT INPUT DISTURBANCE CASES nonlinear and the disturbances in heat duty have altered the entire temperature profile.

3.3 Variable Tray Liquid Holdup

The cases discussed in Section 3.2 were all based on the assumption of constant molar liquid holdup on the trays. Since nonminimum phase behaviour was observed for some responses assuming constant tray liquid holdup it was necessary to rule out the possibility that this assumption was responsible for the observed behaviour. Variable liquid holdup was calculated based on the modified Francis weir equation which is discussed by Wong (1985) and in the DYCONDIST user's manual (Carling, 1986). The equation requires specification of effective weir length, effective tray area and weir height. These parameters were determined based on data published in an earlier study of the tower (Ballard *et al.*, 1978) and are summarized in Table 3.5. Tray holdup values for each stage are listed in Table 3.6.

Feed rate disturbances were chosen for this study because they are considered the most common column disturbance. The responses of interest were product compositions, tray liquid holdup, temperatures and column liquid rates. For consistency with the constant holdup cases, reflux was set at 90 kmol/min and reboiler duty at 500 kJ/min. Constant molar holdup in the condensate receiver and base surge were assumed. Feed composition and initial column conditions were as shown in Table 3.1.

Table 3.5

DEPROPANIZER TRAY DETAILS

Effective Weir length	2.44 m
Effective tray area	6.96 m^2
Weir height	0.046 m
Column diameter	3.66 m

Note: effective tray area was calculated based on the assumption that 75% of the sieve tray area is active (Treybal, 1968).

Table 3.6

BASE CASE TRAY LIQUID HOLDUP

Stage Number	Holdup (kmol)
2	22.0
3	21.8
4	21.5
5	21.1
6	20.5
7	19.8
8	19.0
9	17.9
10	16.8
11	15.8
12	14.8
13	16.0
14	15.9
15	15.7
16	15.5
17	15.2
18	14.9
19	14.6
20	14.2
21	13.8
22	13.4
23	13.0
24	12.8
25	12.5
26	12.3
27	12.2
28	12.1
29	12.0
30	11.9

Figure 3.28 shows the final steady state tray holdup profile for ±10% feed rate disturbances. As discussed in Section 3.1, a constant holdup value of 14 kmol per stage had been previously assumed. Use of the base case holdup distribution shown in Figure 3.28 yields tray holdups which are between 16% lower and 36% higher than the value initially assumed.

The assumption of constant holdup has no affect on the final steady state temperature profile as can be seen in Figure 3.29. The temperature profiles corresponding to the constant and variable holdup cases for a 10% feed rate increase are superimposed as are those for a 10% feed rate decrease. Figures 3.30 shows light and heavy key mole fractions in the distillate and bottoms for ±10% feed rate disturbances in constant and variable holdup cases. There is some variation in the transient values, but the general trends, existence of inverse response, and the final steady state values are independent of the holdup assumption employed.

On the basis of these observations it was decided that constant molar holdup could be assumed for all but the most detailed studies. The base case holdup profile shown in Figure 3.28 is more realistic than the assumption of a constant molar holdup equal for all stages. As discussed in Section 3.1, the disturbance response cases described in Section 3.2 were therefore run using the initial steady state holdup distribution calculated using the variable

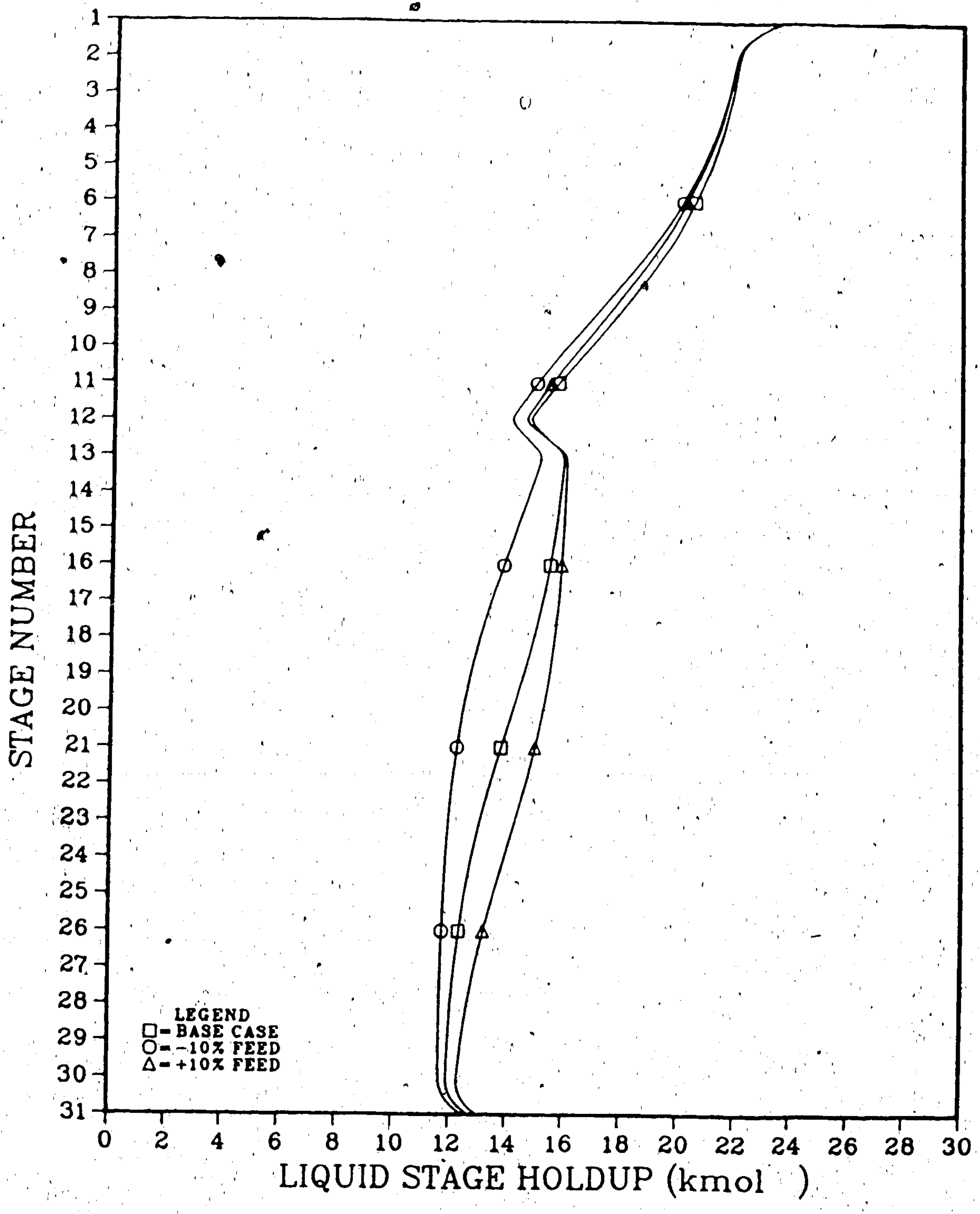


Figure 3.28

STEADY STATE HOLDUP PROFILES FOR 10% FEED DISTURBANCES

MODELLED WITH VARIABLE TRAY HOLDUP

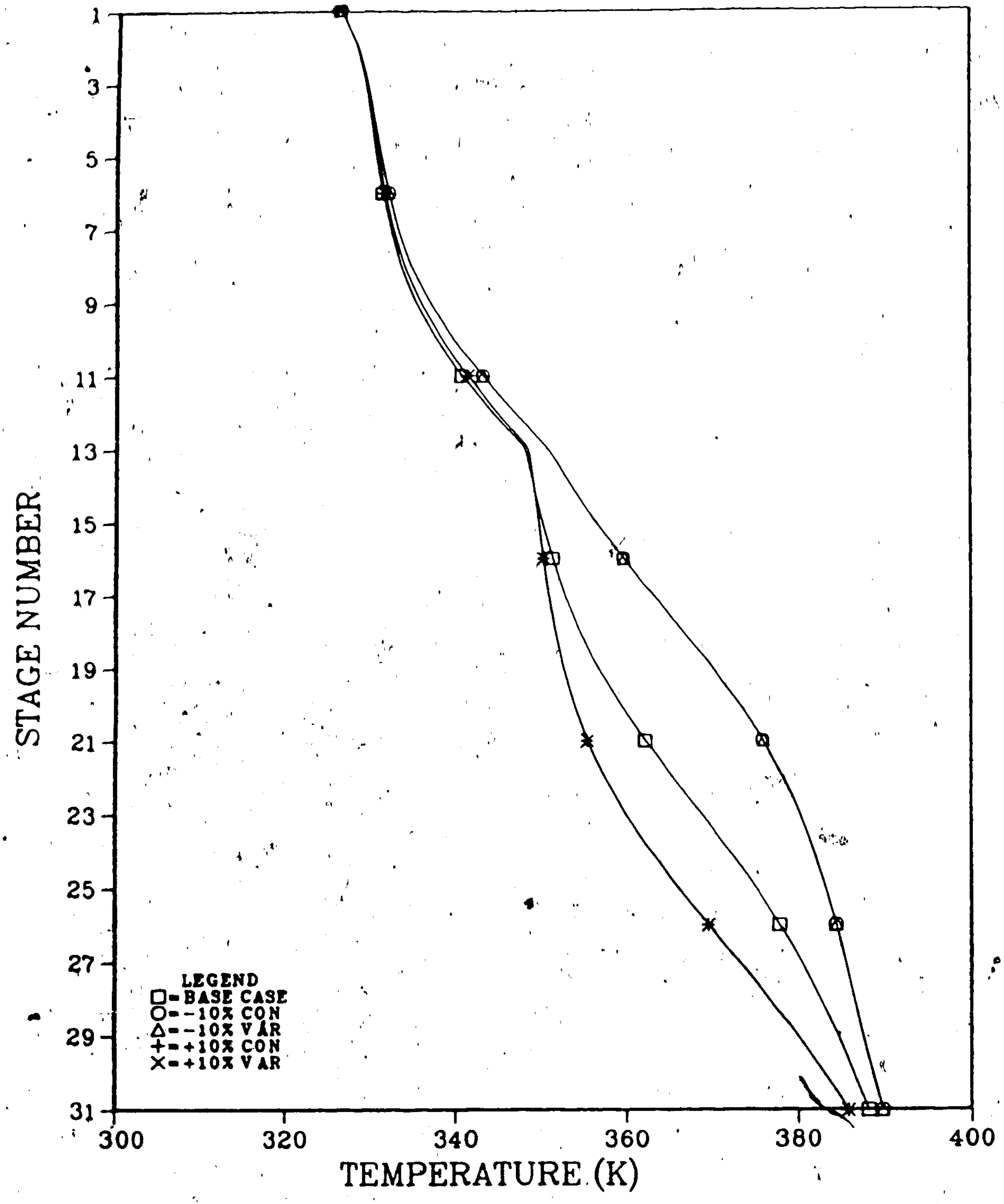


Figure 3.29

STEADY STATE TEMPERATURE PROFILES FOR 10% FEED DISTURBANCES

MODELLED WITH VARIABLE TRAY HOLDUP

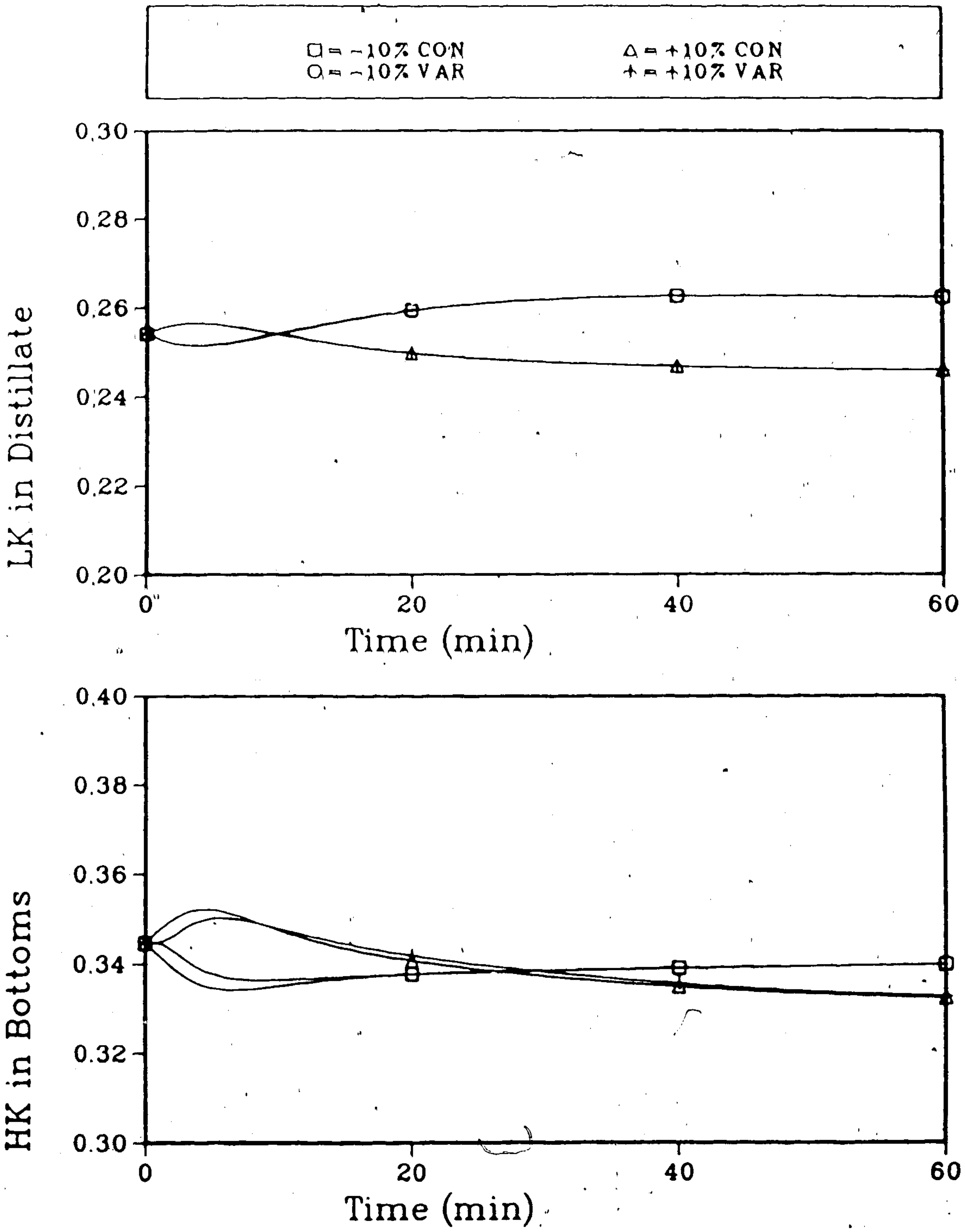


Figure 3.30

KEY COMPONENT RESPONSES IN LIQUID DISTILLATE AND BOTTOMS MODELLED WITH CONSTANT AND VARIABLE TRAY HOLDUP OPTIONS holdup assumption.

3.4 Feed Composition Variation

A series of cases was run to study the effects of both the number of feed components and the feed composition on column dynamics. Base case feed rate, reflux rate, reboiler duty, feed point, and feed temperature were as discussed in Section 3.2. Constant molar tray holdup of 14 kmol was assumed. Feeds with three, four, and five components were investigated. The feed compositions used are summarized in Table 3.7. The base case feed is included for comparison. Five component feed 3D corresponds to the feed composition used by Cook (1980). For most of the cases the mole fractions of the heavy feed components are held constant to examine the effect of variation of the light feed fraction.

A minimum of two cases was run for each feed. The first case corresponded to the determination of the initial steady state conditions. The second case simulated response to a 10% feed rate decrease. The resulting initial and final steady state temperature profiles are grouped by number of feed components and are shown in Figures 3.31 through 3.33. The profiles serve to emphasis the range of operating conditions represented by the feeds for constant reflux rate and reboiler duty.

Due to the results of the base feed dynamic response investigation, instances of inverse response were of special interest. These are summarized for the three, four, and

Table 3.7

FEED COMPOSITIONS FOR FEED VARIATION STUDY

	Component Mole Fraction				
	Ethane	Propylene	Propane	Isobutane	Cisbutene
4 COMPONENT					
Feed 1A	-	0.43	0.15	0.15	0.27
Feed 1B	0.43	-	0.15	0.15	0.27
Feed 1C	-	0.23	0.15	0.35	0.27
3 COMPONENT					
Feed 2A	0.03	0.55	-	-	0.42
Feed 2B	-	0.58	-	0.15	0.27
Feed 2C	-	-	0.58	0.15	0.27
5 COMPONENT					
Feed 3A	0.20	0.23	0.15	0.15	0.27
Feed 3B	0.01	0.42	0.15	0.15	0.27
Feed 3C	0.02	0.41	0.15	0.15	0.27
Feed 3D	0.03	0.20	0.15	0.35	0.27
Base Feed	0.03	0.40	0.15	0.15	0.27

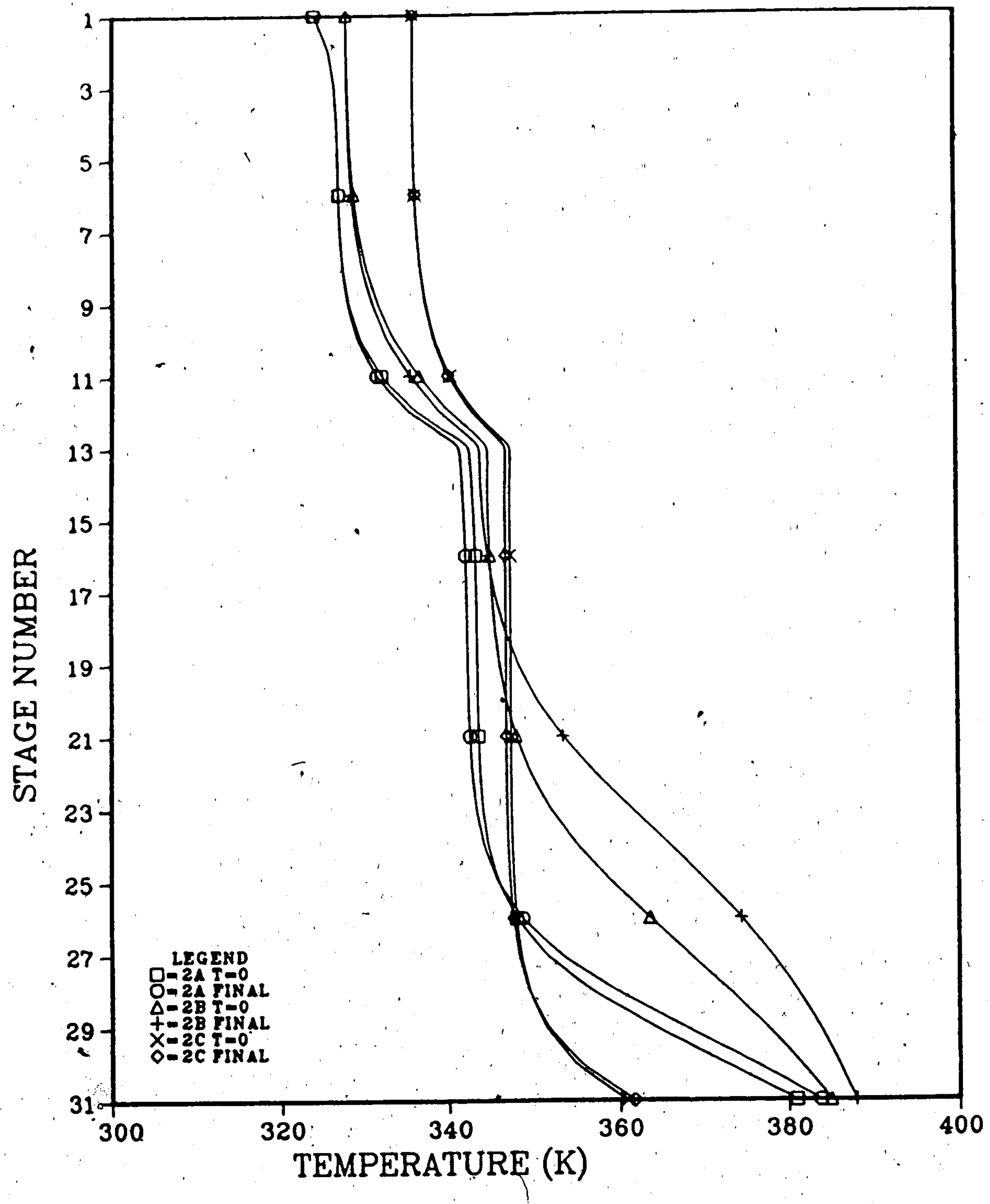


Figure 3.31

STEADY STATE TEMPERATURE PROFILES FOR 3 COMPONENT FEEDS SUBJECTED TO 10% FEED RATE DECREASES

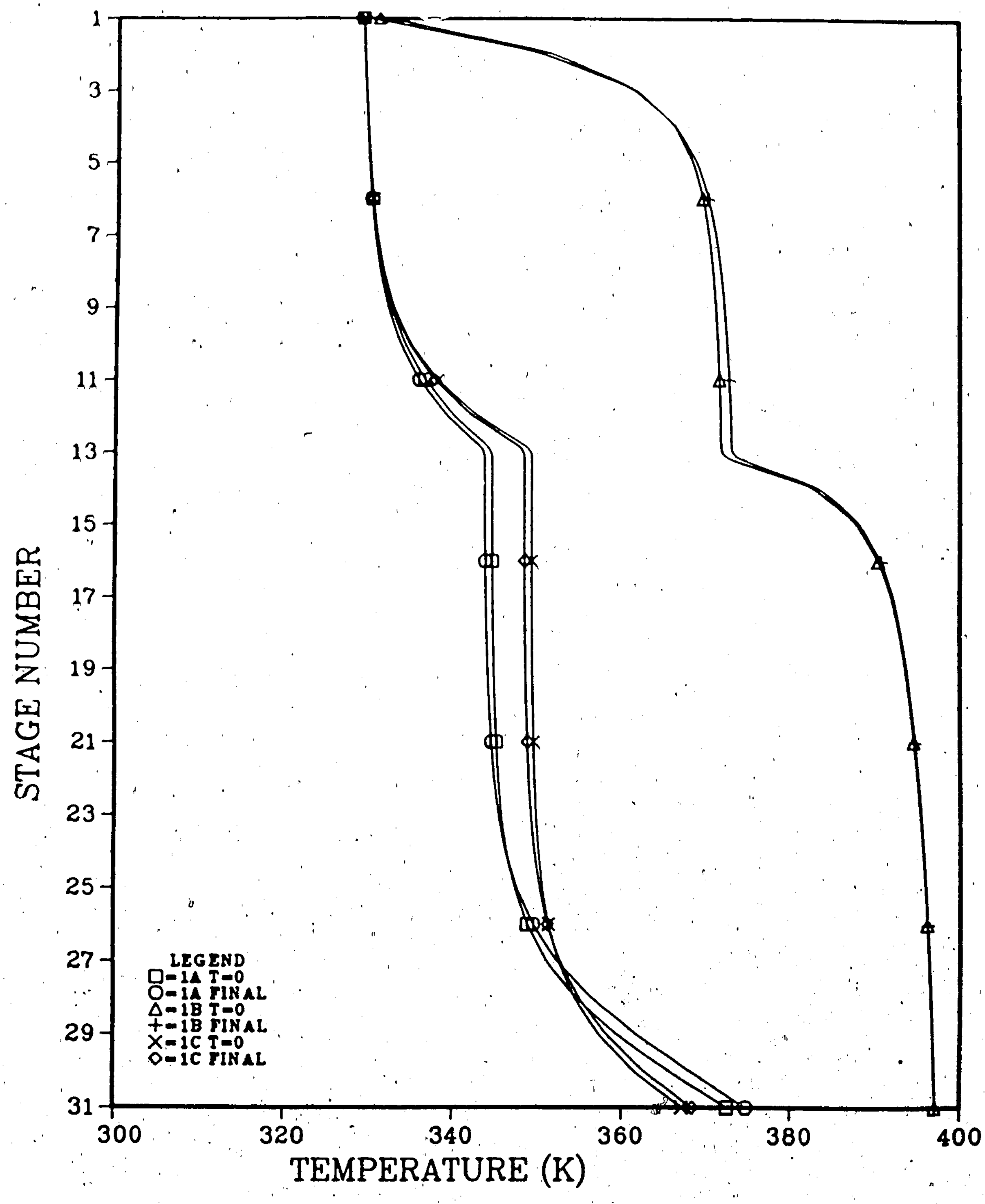


Figure 3.32

STEADY STATE TEMPERATURE PROFILES FOR 4 COMPONENT FEEDS SUBJECTED TO 10% FEED RATE DECREASES

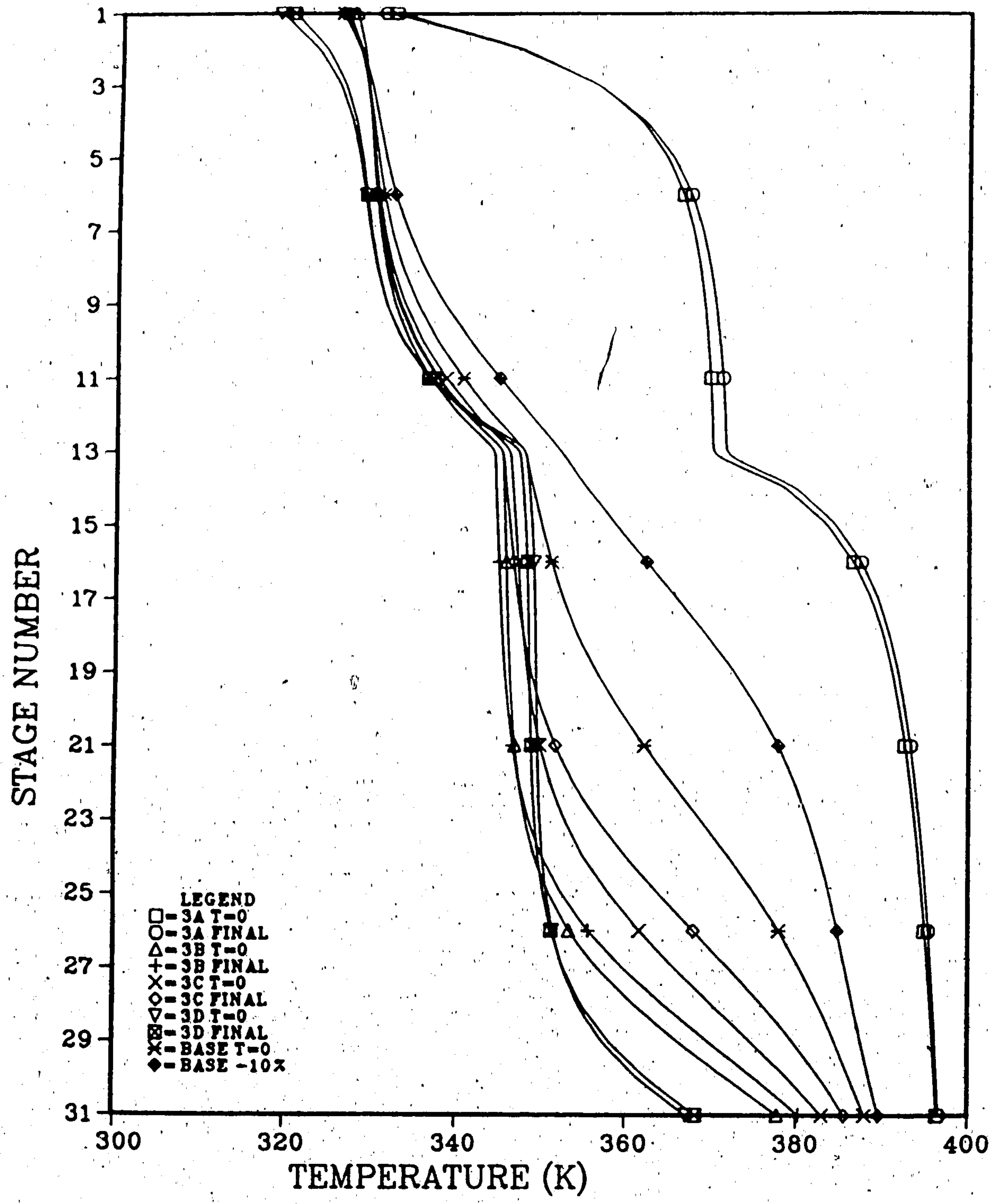


Figure 3.33

STEADY STATE TEMPERATURE PROFILES FOR 5 COMPONENT FEEDS

SUBJECTED TO 10% FEED RATE DECREASES

five component feed streams in Tables 3.8, 3.9 and 3.10 respectively. Limits on the deviations considered when flagging inverse responses were imposed as discussed in Section 3.2.2.

The following general trends may be observed.

- There are more instances of inverse response as the number of system components is increased.
- Inverse stage temperature responses are not observed for three and four component feed cases.

Very small differences in compositions result in unexpected differences in the responses observed. This is exemplified by comparing the series of feeds represented by the four component feed 1A, and five component feeds 3B, 3C, and the base case feed. In this series the mole fractions of propane, isobutane, and cisbutene are held constant. For each successive feed in the series the amount of ethane is increased by one mole percent, while the amount of propylene is decreased. As the feed mole fraction of ethane increases certain patterns can be seen in the tray locations with inverse response. These are considered by component:

- Propylene

  Two zones of inverse propylene response are noted in feed case 1A as is shown in Table 3.11a. These are on stages 1 to 5 and on stage 18. As the amount of C2 in the

Table 3.8

SUMMARY OF INVERSE RESPONSE BEHAVIOUR FOR 3 COMPONENT FEED CASES

CASE	COMPONENT 1	 2	 3	Temperature
Feed 2A				
LK= 2	D			
HK= 3	R-2			
		S-3	S-4	
Feed 2B				
LK= 1	S-1	S-2	S-2	
HK= 2		B		
Feed 2C				
LK= 1	S-3	S-4	S-4	
HK= 2				

LEGEND:

D: liquid distillate product

F: feed stage

B: bottom product

R-x: x rectification stages

S-x: x stripping stages

Table 3.9

SUMMARY OF INVERSE RESPONSE BEHAVIOUR FOR 4 COMPONENT FEED CASES

CASE	COMPONENT				Temperature
	1	2	3	4	
Feed 1A LK= 2 HK= 3		D R-5 S-4	S-4	S-3	
Feed 1B LK= 3 HK= 4	R-1	R-3	D R-1 S-10	S-17 B	
Feed 1C LK= 2 HK= 3	S-1	S-4	D R-6 S-4	R-2 S-4	

LEGEND:

D: liquid distillate product
F: feed stage
B: bottom product
R-x: x rectification stages
S-x: x stripping stages

Table 3.10

SUMMARY OF INVERSE RESPONSE BEHAVIOUR FOR 5 COMPONENT FEED CASES

CASE	C2	C3-	C3	iC4	cC4	Temperature
Feed 3A LK= iC4 HK= cC4	R-1	R-3	R-4	R-3 F S-2	R-3	R-1
Feed 3B LK= C3 HK= iC4	R-1	R-7 S-2	D R-5 S-3	S-2	S-2	
Feed 3C LK= C3 HK= iC4	R-1	R-8 S-3	D R-2	B	S-1	
Feed 3D LK= C3 HK= iC4		R-1 S-1	S-5	R-4 S-4	S-4	
Base Feed LK= C3 HK= iC4	R-1	R-11 F S-1	D R-8 F S-5	D R-11 F S-3	D R-11 F S-4	R-1 F

LEGEND:

D: liquid distillate product

F: feed stage

B: bottom product

R-x: x rectification stages

S-x: x stripping stages

system increases, the number of trays displaying propylene inverse response also increases and the zones extend toward each other.

Table 3.11a
STAGES DISPLAYING INVERSE PROPYLENE RESPONSE

	Zone 1	Zone 2
Feed 1A	1 - 5	18
Feed 3B	1 - 8	17 - 16
Feed 3C	1 - 10	16 - 14
Base Feed	2 - 14	14 - 2

- Propane.

Two zones of inverse propane response may be identified for -10% feed rate disturbances for each feed composition as is summarized in Table 3.11b. One zone, in the rectification section, decreases in size with increasing ethane content in the feed. The second zone varies in size and is located higher in the column for feeds with higher ethane content.

Table 3.11b
STAGES DISPLAYING INVERSE PROPANE RESPONSE

	Zone 1	Zone 2
Feed 1A	1 - 7	29 - 26
Feed 3B	1 - 7	27 - 25
Feed 3C	1 - 6	22
Base Feed	1 - 5	18 - 9

- Isobutane

There are again two zones in which inverse responses are observed and the corresponding stage numbers are shown in Table 3.11c. Both of these are located higher in the column for feeds with high ethane content than for feeds with lower ethane content. The two zones are not apparent in all cases, but the inverse responses which are observed are in agreement with the general trend.

Table 3.11c

STAGES DISPLAYING INVERSE ISOBUTANE RESPONSE

	Zone 1	Zone 2
Feed 1A	23 - 20	—
Feed 3B	21 - 18	—
Feed 3C	—	31
Base Feed	13 - 1	30 - 27

- Cisbutene

A single zone of inverse response is noted with location dependent on the amount of ethane in the feed as shown in Table 3.11d.

Table 3.11d

STAGES DISPLAYING INVERSE CISBUTENE RESPONSE

	Zone 1
Feed 1A	25 -22
Feed 3B	23 - 21
Feed 3C	20
Base Feed	17 - 1

Examination of trends within this series and for the other feed variation cases leads to some further general conclusions:

- Inverse responses tend to occur on adjacent stages.
- The location of the inverse response stages is very sensitive to feed composition.

Consideration of the column profiles in the region of the stages displaying inverse response may provide some further insight. As noted in Section 1.1.5, it has been suggested that irregular behaviour may be expected near an extremum in the composition profiles where system gains are small or near where they change sign (Waller and Gustaffson, 1972). The validity of these criteria can be evaluated by comparing the locations of stages displaying inverse responses given in Tables 3.11 with the composition profiles plotted for each of the feeds in the series in Figures 3.34 through 3.37 for propylene, propane, isobutane, and cisbutene respectively. Consider, for example, the distribution of propane for the various feed cases. From Table 3.11b the rectification section inverse response zone ends on stages 5 to 7 depending on the feed used. In Figure 3.35 the profile extrema do occur on these stages. The same correspondence can be observed for Zone 2 stages for feed cases 1A, 3B, and 3C. The inverse responses on stages 9 - 18 seen in the case of the base case feed do not,

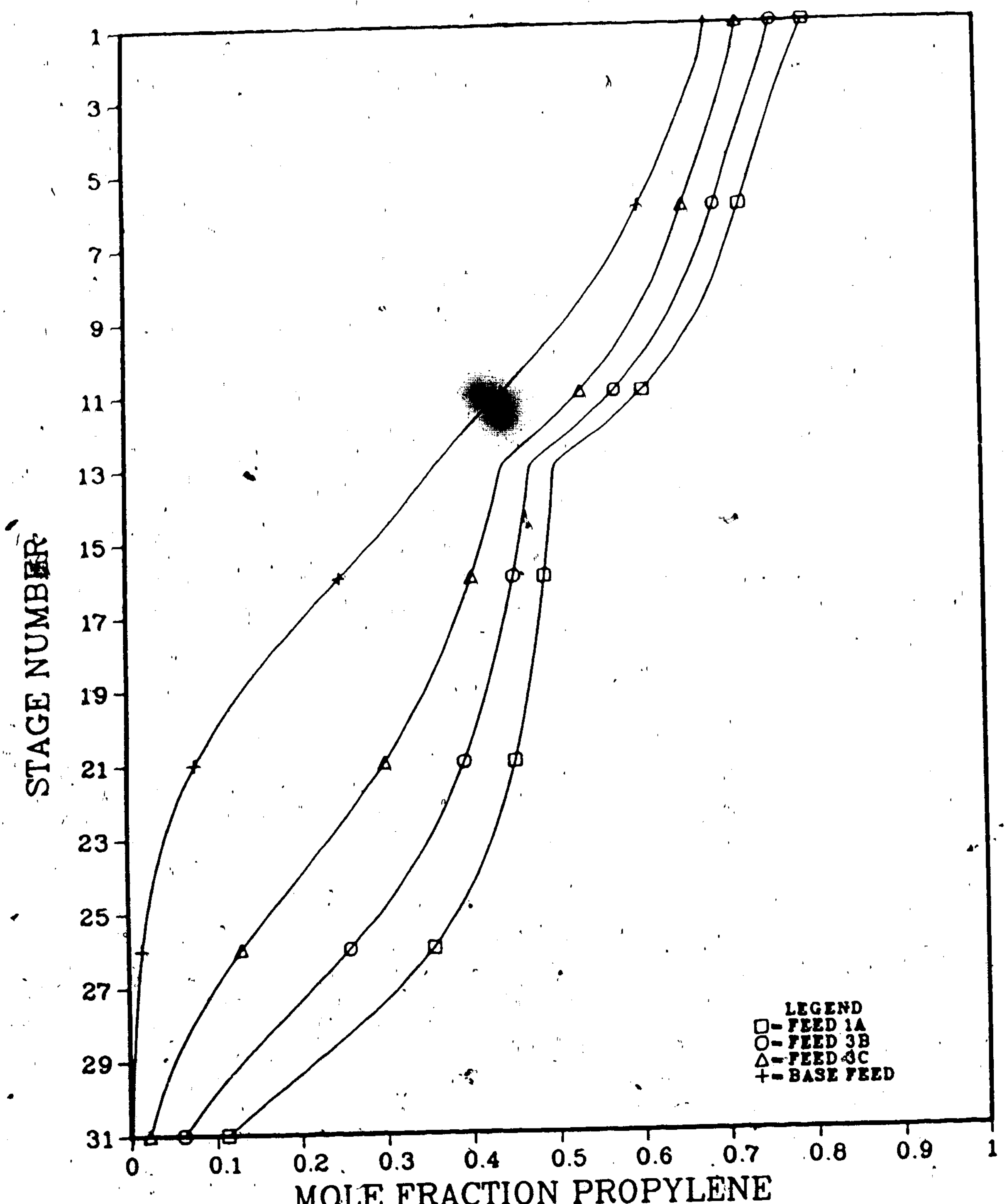


Figure 3.34

PROPYLENE DISTRIBUTION PROFILE AFTER 10% FEED RATE DECREASE FOR FEEDS WITH VARIOUS ETHANE FRACTIONS

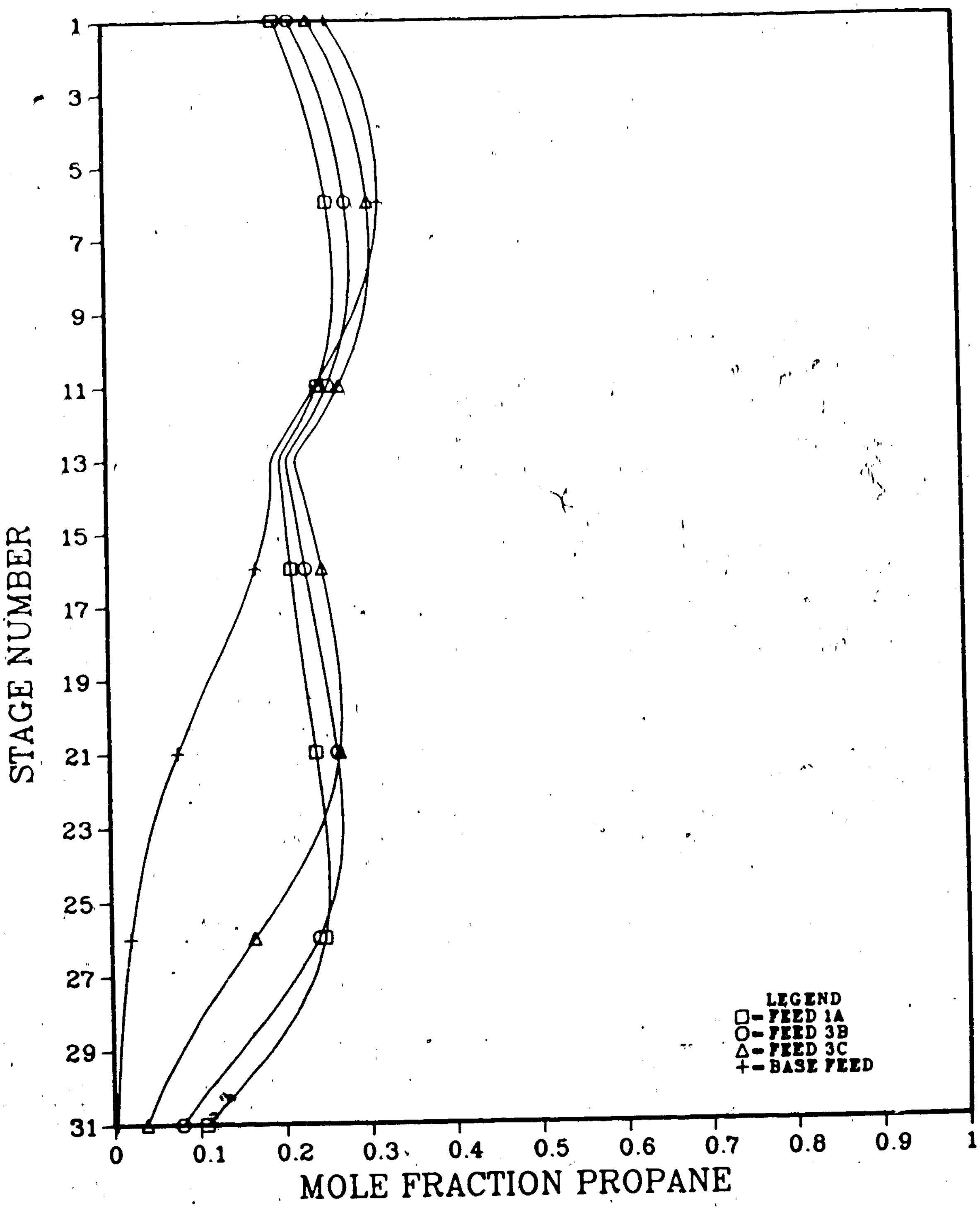


Figure 3.35

PROPANE DISTRIBUTION PROFILE AFTER 10% FEED RATE DECREASE

FOR FEEDS WITH VARIOUS ETHANE FRACTIONS

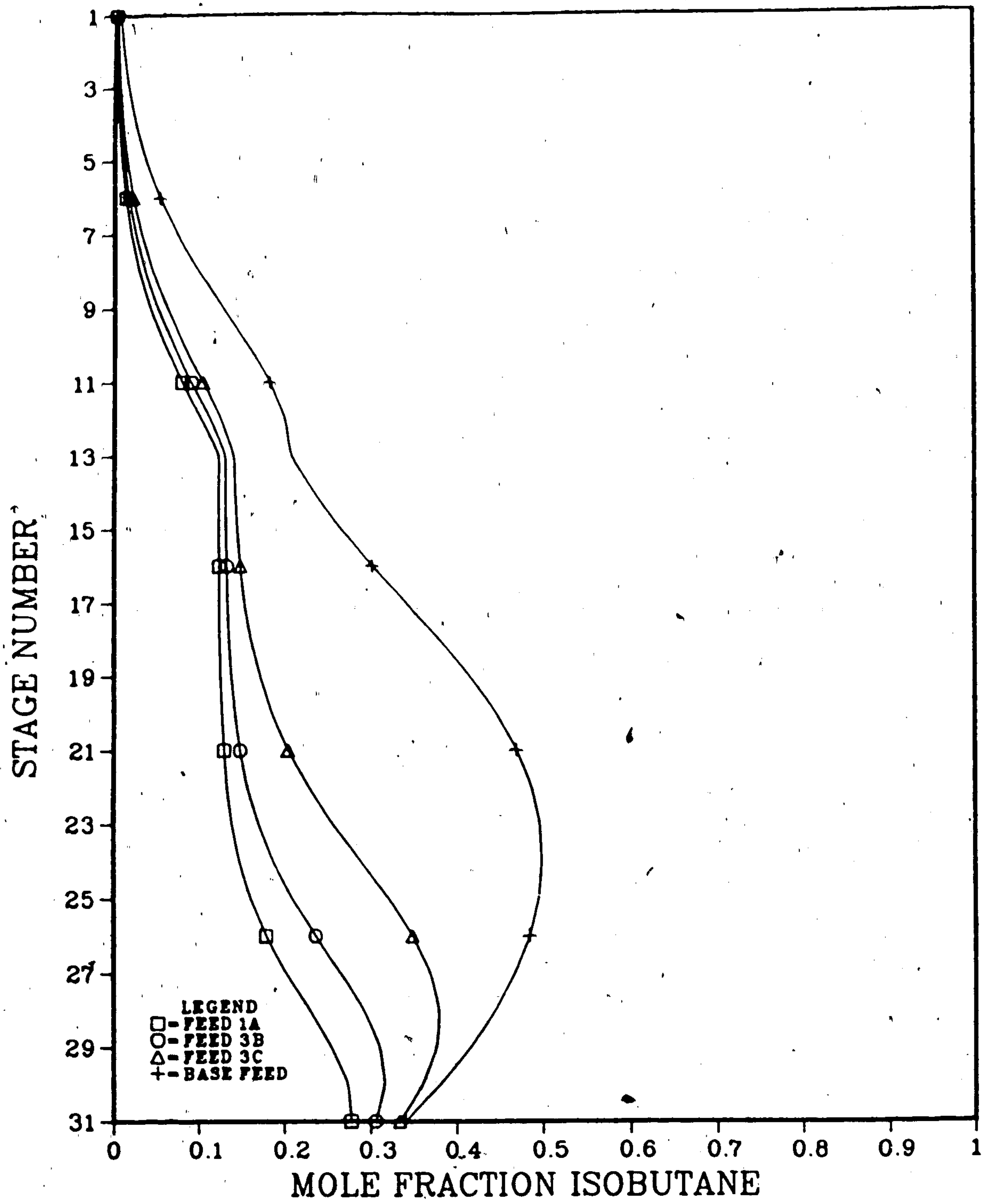


Figure 3.36

ISOBUTANE DISTRIBUTION PROFILE AFTER 10% FEED RATE DECREASE FOR FEEDS WITH VARIOUS ETHANE FRACTIONS

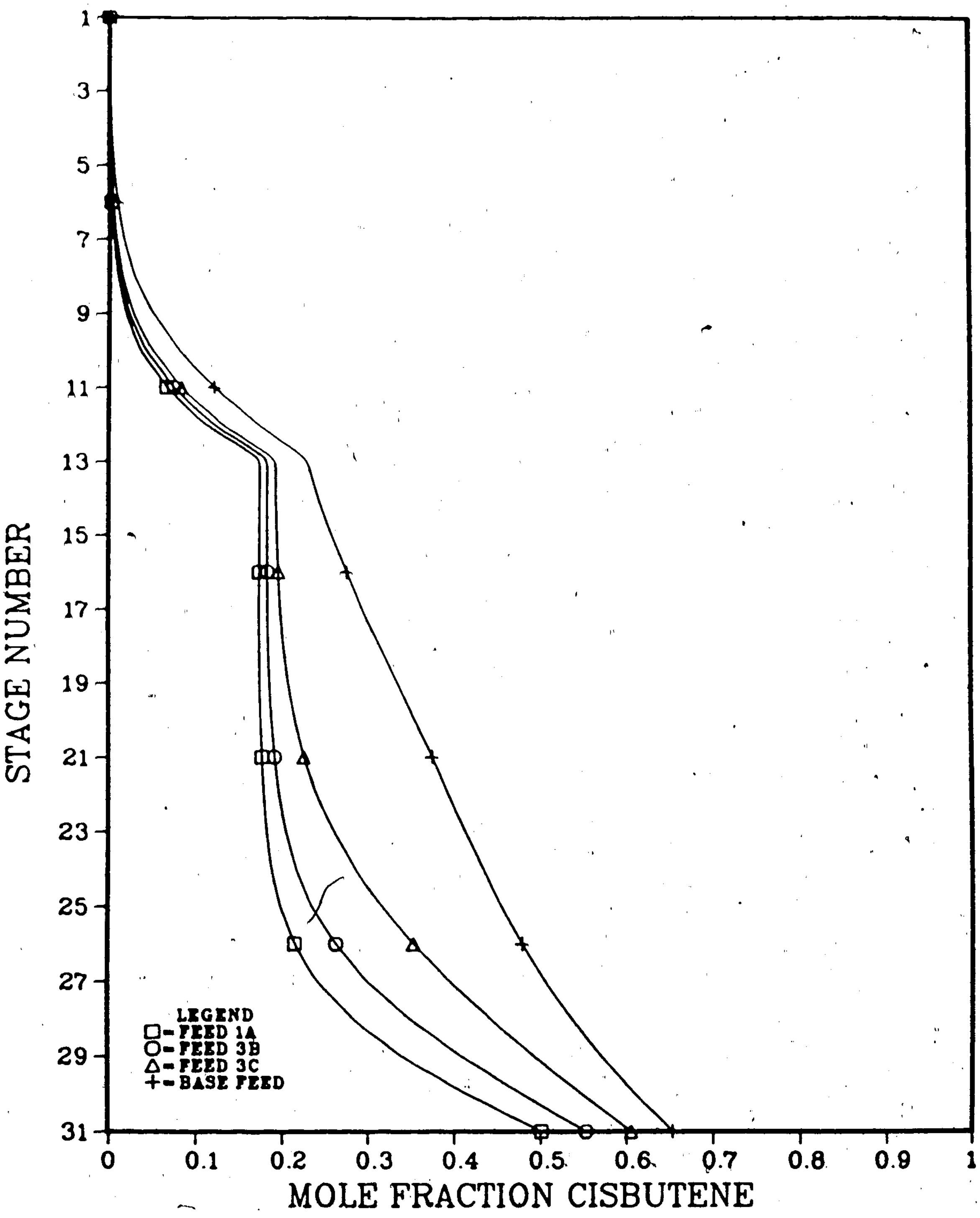


Figure 3.37

CISBUTENE DISTRIBUTION PROFILE AFTER 10% FEED RATE DECREASE

FOR FEEDS WITH VARIOUS ETHANE FRACTIONS

however, follow this pattern. Another exception is seen in Figure 3.34 where inverse propylene response occurs on stages 2 - 14 despite the fact that there is no local extremum in that part of the profile and that the gain, or rate of change of composition with stage number, is not small relative to other portions of the same profile. In fact, using these criteria, one might predict inverse propylene response around stages 21 - 25. This set of criteria appears, then, to be neither necessary nor sufficient for the prediction of inverse response behaviour.

4. SIMULATION OF CONTROL LOOPS

4.1 Problem Description

For closed loop simulation the dynamic model discussed in Chapters 2 and 3 should ideally be treated as a "black box". In other words, control action and process model calculations should be independent. From the point of view of the model, the control action could then be considered as a disturbance in the manipulated variable at the sampling instant. This approach may certainly be used for those discrete loops associated with distillation control. However, some loops should be simulated as continuous and in these cases the "black box" approach fails. This results in some overlap between control and process simulation functions of the simulator.

When incorporating control loops into the simulator it was decided that the continuous controller assumption would be restricted to those local controllers associated with level and flow control about the condensate receiver and column base. All other loops would be handled with discrete controllers. This restriction was necessary in order to limit the number of possible structures of the system equations. Continuous controllers add linkages between variables which were independent in the case of pure column dynamics. For example, if a temperature feedback controller manipulates reflux rate, then the controller links the stage on which the sensor is located with the first column stage where reflux is returned to the tower. In the case of pure dynamics, each stage is affected directly only by those stages above and below it. Not only are the number and locations of the local control linkages dependent on the control strategy selected, but the form of the expression used to describe the relationship is a function of the controller type and parameters. Since the simulator is to be used to evaluate a wide variety of control structures and algorithms, it was not feasible to allow reconfiguration of the system equations to accommodate any and all possible choices.

Some other design features of the control system aspects of the simulator are discussed below. These were considered at each stage of the software development in order to minimize development time and effort.

- <u>Flexibility</u>

  Flexibility to model a variety of control system structures is required as is flexibility to consider all possible manipulated and controlled variables. For example, it should be possible to evaluate performance of schemes employing a temperature difference or other function of two or more temperatures as the controlled variable.

- Expandability

  The approach taken for design should be to incorporate conventional structures and algorithms initially while maintaining the option of adding advanced and/or unconventional schemes later. The incremental approach permits debugging of each level before moving to the next, more complex, level.

- Style

  The simulator is a large and complex software package. Its maintenance will be simplified if the control additions are written in a manner consistent with the existing code.

4.2 Local Control Loops

As discussed in the previous section, local controllers will be simulated in a continuous form only. The control action must then be calculated at each step of the integration to approximate a continuous controller output. The initial approach taken was to use a common step size for the simulation of column dynamics and local controllers. The future addition of the option of using a smaller step size for the local controller simulation was also considered.

4.2.1 Local Level Control

Local level control affects the calculation of the Jacobian used in the integration of the overall material balance described by Equation 2.1. The system of equations resulting from one choice of control strategy is developed in Section 4.2.3.

It should be noted that proportional-only, (P-only), controllers have been selected for level control to simplify calculations. The complexity of modelling proportional-integral, (PI), level controllers is illustrated in the example of Section 4.2.3. The assumption of P-only level controllers is not unrealistic. The controllers are simple, inexpensive and almost foolproof (Buckley *et al.*, 1985). There are, however, limitations. A larger accumulator drum is required to obtain the same amount of flow smoothing with P-only level control as could be obtained with a PI controller. The code could be modified to simulate PI level controllers if a detailed study of material balance control were required.

4.2.2 Local Flow Control

Flow controllers can be simulated in either local or remote mode. In local mode continuous P or PI controllers can be simulated. In remote mode any control algorithm can be employed or the controlled variable can be fixed. The latter option is equivalent to assuming perfect control of the flow. In this case it must be assumed that the dynamics of the flow loop are much faster than the other process and control system dynamics.

4.2.3 Local Control Example

This example deals with the integration of the overall material balance equations written for the top of the column when local controllers are in effect. The control structure assumed is shown in Figure 4.1. Liquid distillate is assumed to be on flow control while the reflux rate is manipulated to control accumulator level.

Considering the material balance around the condenser and accumulator drum, stage 1, for

$F_1 = L_0 = S_1 = 0$

$s_1 = D$

where D is the molar liquid distillate flow rate, the material balance equation may be written as:

$$\frac{dM_1}{dt} = V_2 - V_1 - L_1 - D \tag{4.1}$$

The controller equations for the reflux and liquid distillate may also be written. If a P-only controller is assumed for the level loop then

$$L_1 = K_p(z^{SP}-z) + L_{1,bias} \tag{4.2}$$

Alternatively, if PI control is assumed, then

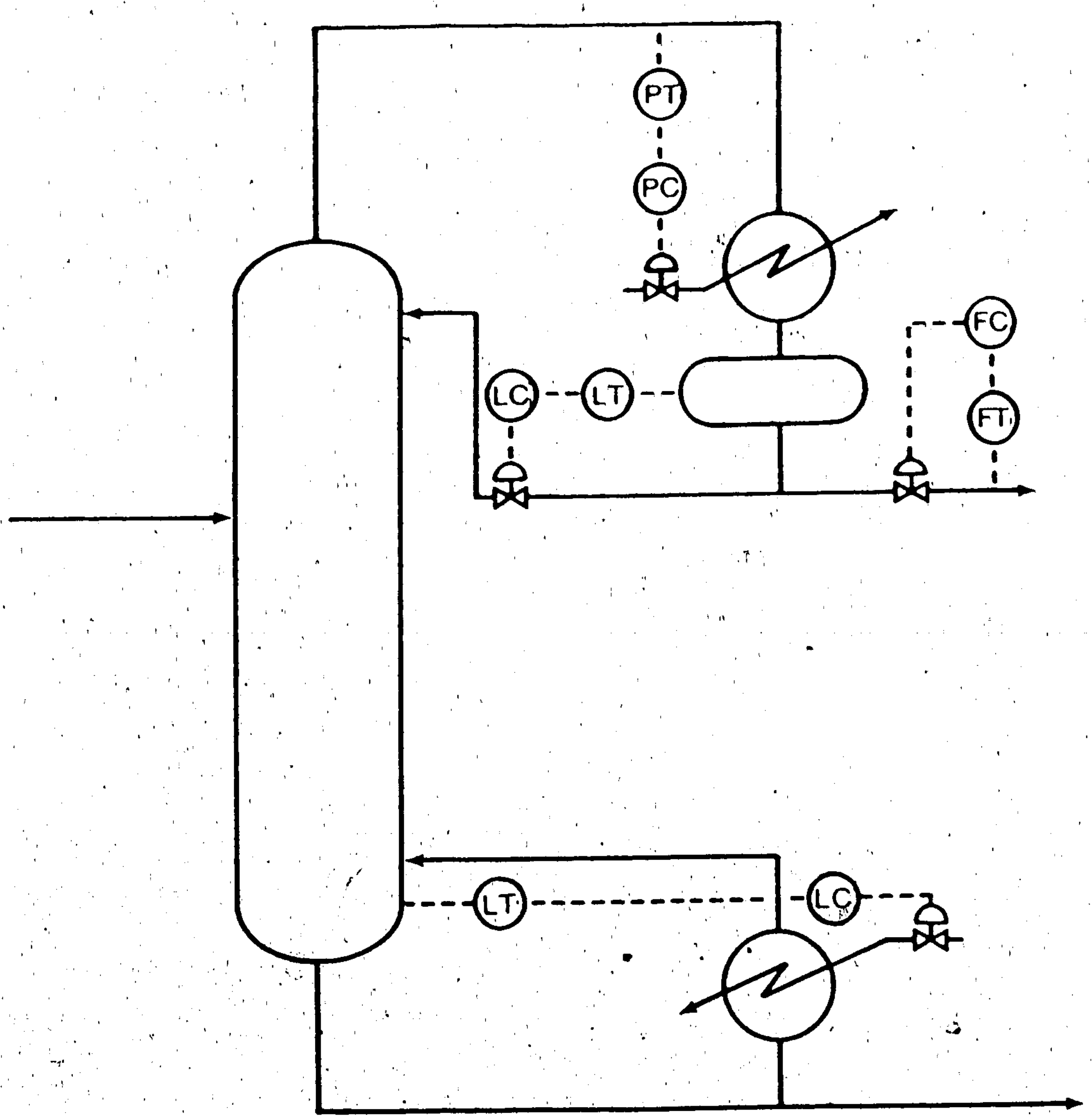


Figure 4.1

MATERIAL BALANCE CONTROL FOR LOCAL CONTROL EXAMPLE

$$L_1 = K_p \left\{ (z^{SP}-z) + K_i \int_0^t (z^{SP}-z)dt \right\} + L_{1,bias} \qquad (4.3)$$

In both cases the sign of the gain term must be negative to ensure the correct control action. For the flow controller, PI control is assumed:

$$OP = K_{p2} \left\{ (D^{SP}-D) + K_{i2} \int_0^t (D^{SP}-D)dt \right\} + D_{bias} \qquad (4.4)$$

The material balance to be integrated then requires the substitution of Equation 4.4 and either 4.2 or 4.3 into Equation 4.1.

In applying the ASIRK integration formulae summarized in Table 2.2, the following assignments are made:

$$y = [M_1 \quad D \quad L_2 \quad \ldots \quad]^t \qquad (4.5)$$

and

$$f\{y\} = [\ \frac{dM_1}{dt} \quad \frac{dD}{dt} \quad \ldots \quad]^t \qquad (4.6)$$

The vector of liquid rates, y, used for the case without local level control is augmented with the molar accumulator and column base holdups. The reflux rate, L_1, is replaced by the liquid distillate rate since the reflux rate may be calculated once the molar accumulator holdup and distillate rate are known. The elements of the Jacobian used to calculate the incremental functions, k_1 and k_2, are:

$$\frac{\partial}{\partial M_1}\left(\frac{dM_1}{dt}\right); \quad \frac{\partial}{\partial M_1}\left(\frac{dD}{dt}\right); \quad \frac{\partial}{\partial D}\left(\frac{dM_1}{dt}\right); \quad \frac{\partial}{\partial D}\left(\frac{dD}{dt}\right)$$

These can be determined from Equations 4.1 through 4.4. If Equation 4.2 is used:

$$\frac{\partial}{\partial M_1}\left(\frac{dM_1}{dt}\right) = K_p\left(\frac{dz}{dM_1}\right) \tag{4.7}$$

If Equation 4.3 is used:

$$\frac{\partial}{\partial M_1}\left(\frac{dM_1}{dt}\right) = K_p\left[\frac{dz}{dM_1} + \frac{\partial}{\partial M_1}\int_0^t (z^{SP}-z)dt\right] \tag{4.8}$$

It is the awkwardness of including the evaluation of the partial derivative of the integral term in Equation 4.8 that resulted in the decision to use P-only level controllers. Equation 4.2 will be used to describe the level controller for the remainder of this example.

Differentiating Equation 4.4 with respect to time yields:

$$\frac{dD}{dt} = -K_{p2}\left(\frac{dD}{dt}\right) + K_{p2}K_{i2}(D^{SP} - D)$$

Hence

$$\frac{\partial}{\partial M_1}\left(\frac{dD}{dt}\right) = 0 \tag{4.9}$$

and

$$\frac{\partial}{\partial D}\left(\frac{dD}{dt}\right) = \frac{-K_{p2}K_{i2}}{1 + K_{p2}} \tag{4.10}$$

Also, from Equation 4.1:

$$\frac{\partial}{\partial D}\left(\frac{dM_1}{dt}\right) = -1 \tag{4.11}$$

The matrix equation used to solve for the set of incremental functions may then be formed. Considering only the upper left corner of the Jacobian and the first two elements of the vectors yields:

$$\begin{bmatrix} 1 - ha\left(K_p\frac{dz}{dM_1}\right) & -ha & \cdots \\ 0 & 1+ha\left(\frac{K_{p2}K_{i2}}{1 + K_{p2}}\right) & \cdots \\ \vdots & \vdots & \vdots \end{bmatrix} \begin{bmatrix} k_{M,1} \\ k_{D,1} \\ \vdots \end{bmatrix} \doteq \begin{bmatrix} \frac{dM_1}{dt} \\ \frac{dD}{dt} \\ \vdots \end{bmatrix} \tag{4.12}$$

so the liquid holdup and distillate rate may be determined at the same time as the column liquid rates.

4.3 Remote Control Loops

Simulation of remote control loops is possible in a discrete form since the control calculations represent an independent program module as was shown in Figure 2.3. The current version of the simulator incorporates both proportional-integral-derivative (PID) and self-tuning (STC) controller types but other user algorithms may also be interfaced if desired. Detailed notes on the use of these algorithms are given in the user manual (Carling, 1986). Some of the general features will be outlined below.

4.3.1 PID Control

The controller output for PID control loops is determined using the following equation.

$$OP = K_p \left[ER + K_i \int_0^t ERdt + K_d \frac{d(MS)}{dt} \right] + BIAS \qquad (4.13)$$

It should be noted that the integral constant has units of $\frac{\text{repeats}}{\text{min}}$ so that integral action is turned off when $K_i=0$. Derivative action is performed on the measurement only avoid the "derivative kick" otherwise associated with a setpoint change. A bias term is added since normalized variables are not used throughout. User-specified high and low control action limits are imposed on the output.

4.3.2 Self-Tuning Control

The self-tuning control algorithm used in this work has recently been discussed by Langman (1987). The algorithm includes options for feedforward and decoupling compensation and can be used with multirate sampling. The derivation of the controller will not be dealt with here, but a brief summary of some of the controller features will be given to establish inherent assumptions as well as the nomenclature used.

The generalized multi-input, multi-output (MIMO) control law is derived based on the assumption that the following z domain representation is valid for a process with vector outputs, $Y(t)$; control action vector, $U(t)$; measurable disturbances, $V(t)$; and which is subjected to random noise inputs, $\Xi(t)$.

$$A(z^{-1})Y(t) = B(z^{-1})U(t) + C(z^{-1})\Xi(t) + D(z^{-1})V(t) \qquad (4.14)$$

The matrices A, B, C and D are polynomial matrices in (z^{-1}). System delays, $z^{-k_{ij}}$ and $z^{-d_{ij}}$, are defined respectively as the delay between the i^{th} control input and the j^{th} process output, and that between the i^{th} measurable disturbance and the j^{th} process output and are included in the matrices B and D as appropriate (Tham *et al.*, 1985).

The control law is calculated by minimizing a cost function including weightings on the system outputs, setpoints and control action. The weightings are provided by $P(z^{-1})$, $R(z^{-1})$ and $Q(z^{-1})$ polynomial matrices respectively. The resulting control law is given by:

$$[z^{k_{ii}-k_{ij}}\hat{G}+Q]U(t) =$$
$$RW(t) - P_d\hat{F}Y(t) - z^{k_{ii}-k_{ij}}\hat{L}V(t) - \hat{H}PY^*(t+k_{ii}-1 \mid t-1) \tag{4.15}$$

The choice of the number of coefficients in the polynomials has been discussed by Langman (1987) and depends on both the system order and delays. The polynomial matrices G, F, L and H are related to the system matrices in Equation 4.14 using the diophantine identity. The polynomial coefficients are estimated recursively and the estimates are used to form the estimated matrices $\hat{G}$, $\hat{F}$, $\hat{L}$ and $\hat{H}$ which are used in Equation 4.15. The estimation algorithm used is a recursive least squares method with upper diagonal factorization (Langman, 1987).

5. CLOSED LOOP SIMULATION EXAMPLE

5.1 Introduction

A closed loop simulation study of the depropanizer studied in Chapter 3 is discussed in this chapter. The objectives of the study were to ensure that the simulator control options were in place and working rather than to optimize the tower control performance. As a result, controller parameters were tuned to yield reasonable rather than optimal control results.

The approach taken was to work from the most elementary control schemes towards more complex strategies. Thus the first control cases involved material balance control alone. These cases are discussed in Section 5.2. Single quality control was studied with the control objective assumed to be first the liquid distillate product composition and then the bottom product composition. Perfect material balance control was assumed. A transition was made from indirect quality control to direct quality control as cases based on temperature feedback were compared with those based on composition feedback. Section 5.3 contains a discussion of these cases and the simulation results obtained. Dual quality control cases are discussed in Section 5.4. Both direct and indirect control strategies were examined and the performance of these schemes was compared. Interaction observed between the two quality control loops led to a study of the amount of interaction predicted based on steady state interaction analysis. This is also discussed in Section 5.4.

Advanced control strategies considered in this work were feedforward control and self-tuning control. Feedforward control action was implemented in conjunction with single quality control and is discussed in Section 5.5. Self-tuning control was implemented a means for dual quality control and is discussed in Section 5.6.

5.2 Material Balance Control

Material balance control cases simulated for this work involved the manipulation of liquid distillate rate to control accumulator level and the manipulation of bottoms rate to control base surge level. Reflux rate was assumed to be on flow control. A diagram of the scheme is given in Figure 5.1. Ideal pressure control was assumed for all cases. Initial operating conditions and column configuration were as discussed in Section 3.1 apart from the use of a total condenser in place of the partial condenser. This substitution was made to simplify computation. Variable tray holdup calculations were based on the Francis weir equation with tray details as summarized in Table 3.5. Constant relative froth density of 1.0 was assumed. The transient calculation of reboiler and base surge holdups was accomplished by augmenting the set of differential equations used to calculate column liquid rates with the molar accumulator holdup, reflux rate and base

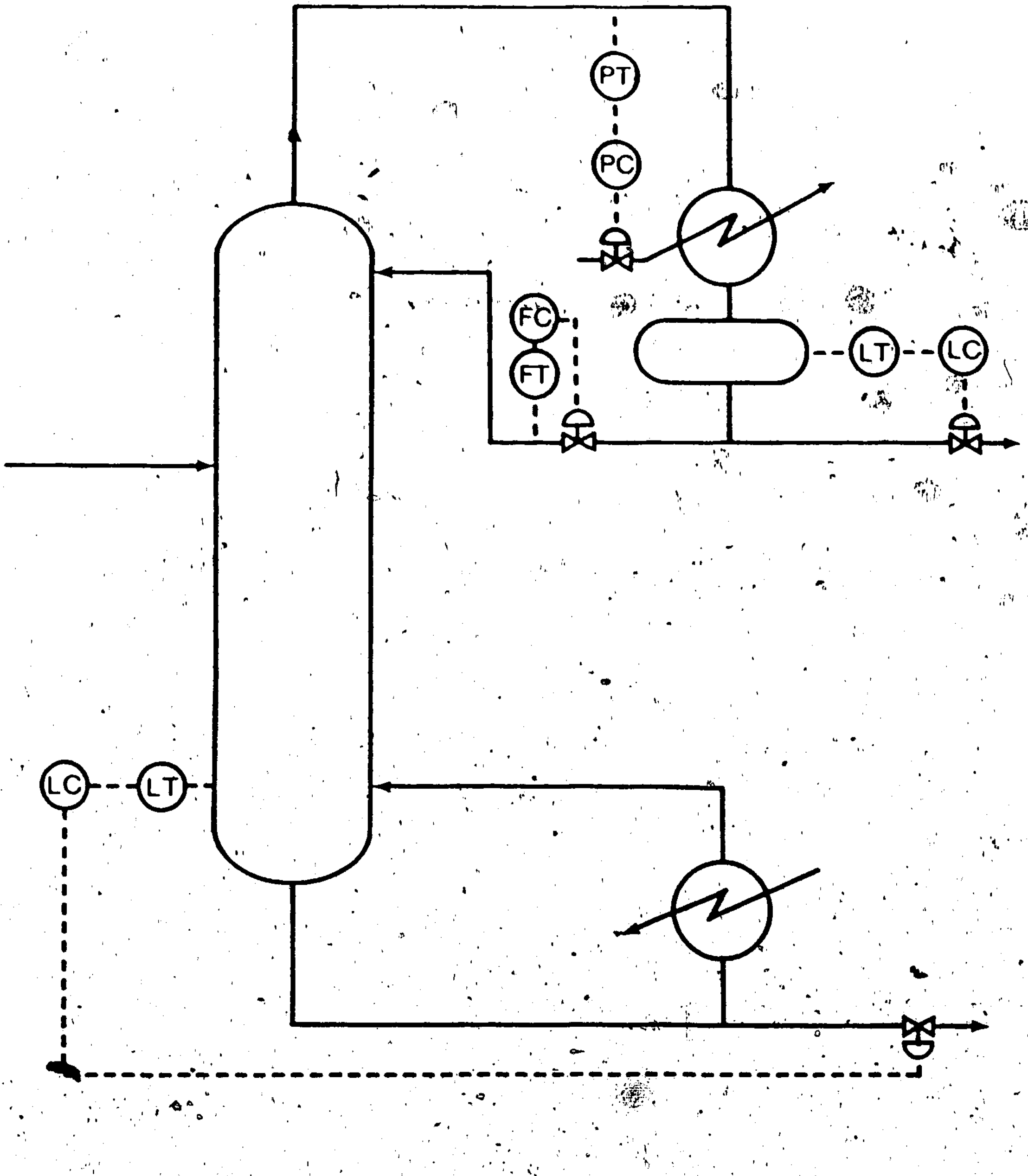


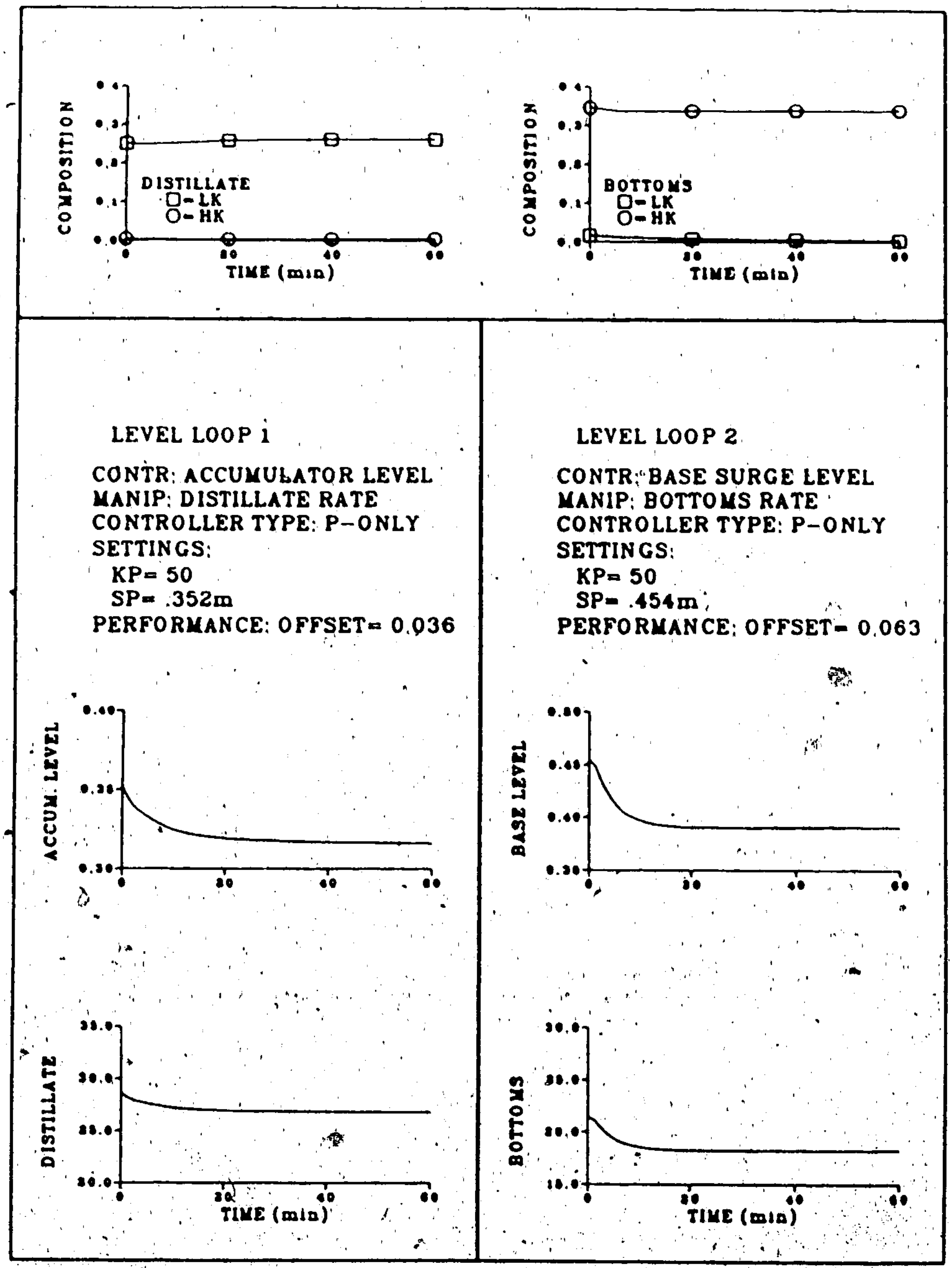
Figure 5.1

MATERIAL BALANCE CONTROL SCHEME

surge molar holdup. The procedure is similar to that used in the local control example discussed in Section 4.2.

For the material balance control cases as for most of the closed loop cases, feed rate decreases of 10% were used to test and tune the controllers. Proportional-only controllers were used. The controller gains used for both loops in cases with column responses plotted in Figures 5.2, 5.3 and 5.4 are 50, 200, and 400 respectively. As noted in Chapter 4, the PID controller equation is not in a normalized form so the parameter values depend on the units of the controlled and manipulated variables.

The format of Figures 5.2 through 5.4 is common to those used to display the results of most of the closed loop cases. The top two trend plots in each figure show the light and heavy key mole fraction responses in the distillate and bottoms products respectively. The remainder of each figure is divided into two sections with one for each of the two control loops of interest. In the case of Figure 5.2, for example, the material in the frame on the left side of the figure pertains to the accumulator level control loop. The settings and a performance index are shown as are two trend plots. The upper plot shows the controlled variable response to the disturbance. The lower plot shows the control action on the manipulated variable, in this case the distillate flow rate. The trend plots are scaled in the following units: time in minutes; composition as mole fractions; level in metres; and flow rates as molar



LEVEL LOOP 1

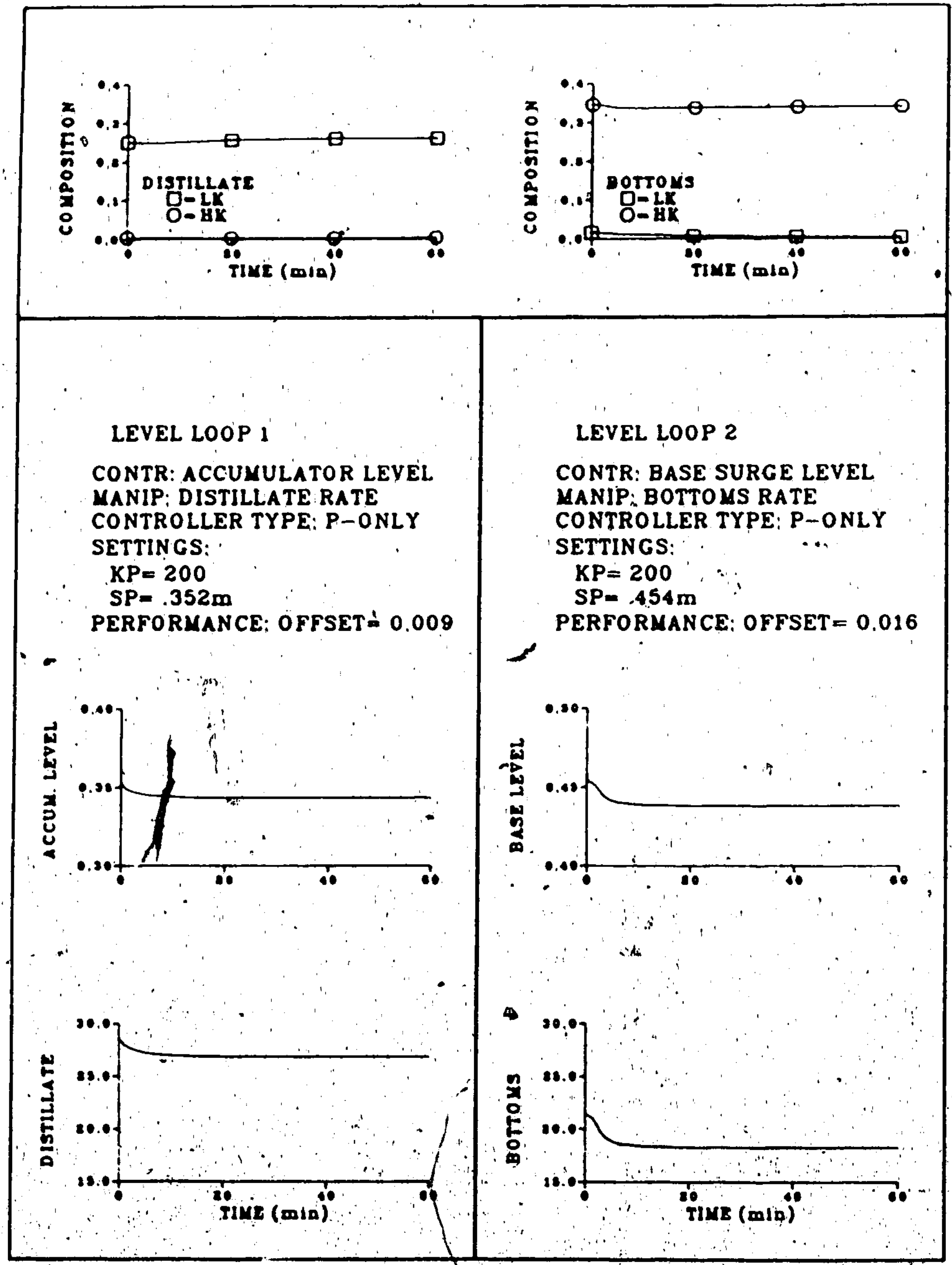
CONTR: ACCUMULATOR LEVEL
MANIP: DISTILLATE RATE
CONTROLLER TYPE: P-ONLY
SETTINGS:
KP= 50
SP= .352m
PERFORMANCE: OFFSET= 0.036

LEVEL LOOP 2

CONTR: BASE SURGE LEVEL
MANIP: BOTTOMS RATE
CONTROLLER TYPE: P-ONLY
SETTINGS:
KP= 50
SP= .454m
PERFORMANCE: OFFSET= 0.063

Figure 5.2

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR MATERIAL BALANCE CONTROL WITH K_p =50



LEVEL LOOP 1

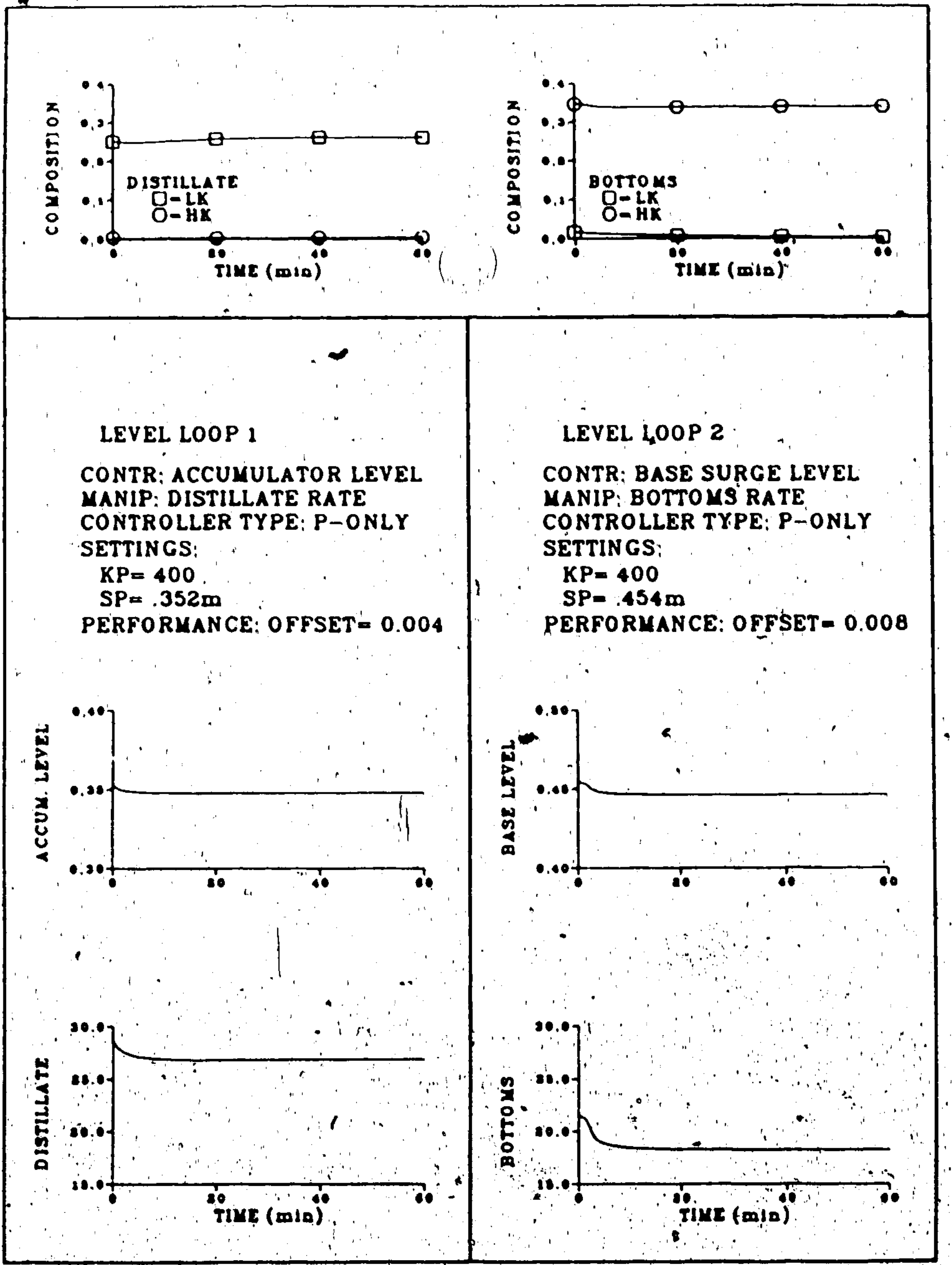
CONTR: ACCUMULATOR LEVEL
MANIP: DISTILLATE RATE
CONTROLLER TYPE: P–ONLY
SETTINGS:
KP= 200
SP= .352m
PERFORMANCE: OFFSET= 0.009

LEVEL LOOP 2

CONTR: BASE SURGE LEVEL
MANIP: BOTTOMS RATE
CONTROLLER TYPE: P–ONLY
SETTINGS:
KP= 200
SP= .454m
PERFORMANCE: OFFSET= 0.016

Figure 5.3

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR MATERIAL BALANCE CONTROL WITH K_p =200



LEVEL LOOP 1

CONTR: ACCUMULATOR LEVEL
MANIP: DISTILLATE RATE
CONTROLLER TYPE: P-ONLY
SETTINGS:
KP= 400
SP= .352m
PERFORMANCE: OFFSET= 0.004

LEVEL LOOP 2

CONTR: BASE SURGE LEVEL
MANIP: BOTTOMS RATE
CONTROLLER TYPE: P-ONLY
SETTINGS:
KP= 400
SP= .454m
PERFORMANCE: OFFSET= 0.008

Figure 5.4

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR MATERIAL BALANCE CONTROL WITH K_p =400

rates per minute (kmol/min).

In all three of the cases shown in Figures 5.2 through 5.4 a 10% feed rate decrease was introduced at the start of the simulation. Noting the criterion that level control should yield smooth and gradual flow rate changes (Buckley *et al.*, 1985), the controlled performance shown in Figure 5.4 represents a good compromise between a fast response and gradual flow changes. Controller gains of K_p= 200 were therefore selected for the mass balance control scheme. These settings were used to test the closed loop response to changes in level setpoint and to a feed rate increase disturbance. The results for these cases are shown in Figures 5.5 and 5.6 respectively. The controllers perform reasonably well for both servo and regulatory control. Smoother control could be obtained in the setpoint change case shown in Figure 5.5 by ramping the setpoint to the desired value rather than making a step change. As was noted in Section 4.3, the controller output is bounded for all cases. In the feed rate increase case for which the response is shown in Figure 5.6, the upper limit for the accumulator level controller should have been set higher to allow faster response since the accumulator level has not reached the new steady state value at the end of the one hour transient. If there were a reason that the distillate rate could not exceed the specified bound, then the distillate stream would represent a column bottleneck and another material balance scheme would be more appropriate.

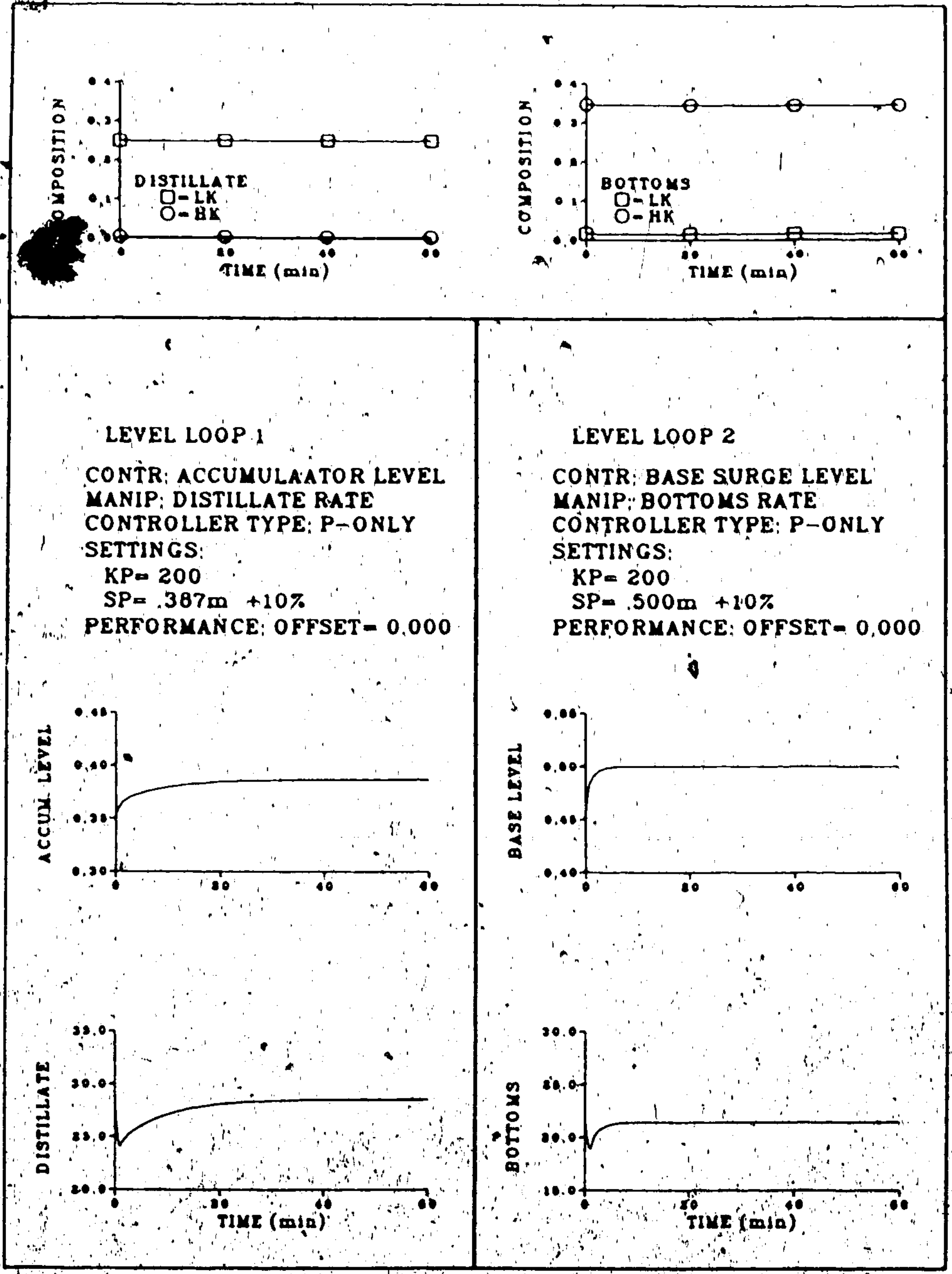
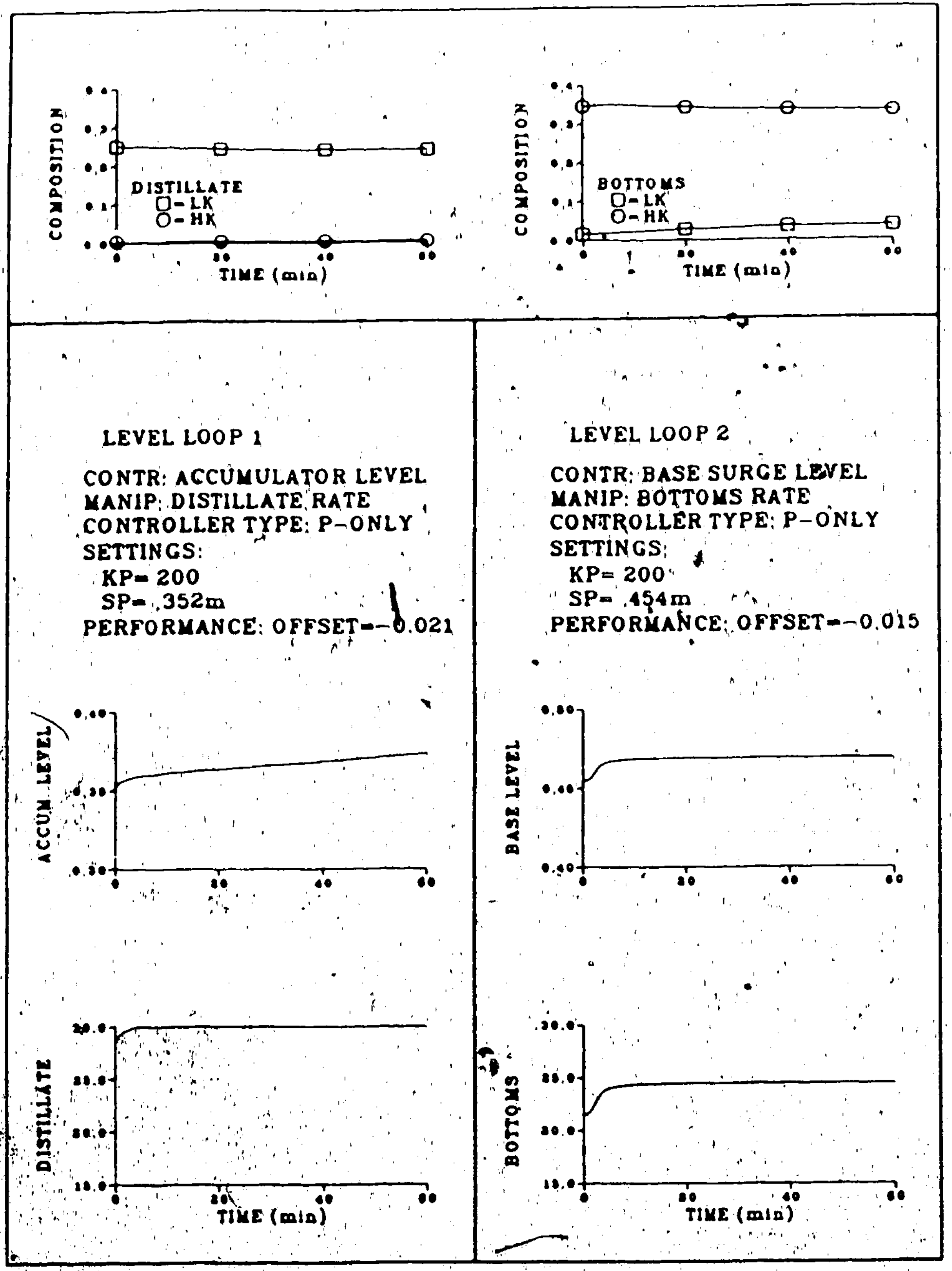


Figure 5.5

CLOSED LOOP RESPONSES TO INCREASES IN LEVEL SETPOINTS FOR MATERIAL BALANCE CONTROL WITH K_p =200



LEVEL LOOP 1
CONTR: ACCUMULATOR LEVEL
MANIP: DISTILLATE RATE
CONTROLLER TYPE: P-ONLY
SETTINGS:
KP= 200
SP= .352m
PERFORMANCE: OFFSET=-0.021

LEVEL LOOP 2
CONTR: BASE SURGE LEVEL
MANIP: BOTTOMS RATE
CONTROLLER TYPE: P-ONLY
SETTINGS:
KP= 200
SP= .454m
PERFORMANCE: OFFSET=-0.015

Figure 5.6

CLOSED LOOP RESPONSES TO A 10% FEED RATE INCREASE FOR MATERIAL BALANCE CONTROL WITH K_p =200

Appropriate control bounds are essential to the success of any control strategy. The base level controller is seen to respond well to the same disturbance.

5.3 Single Quality Control

5.3.1 Temperature Sensor Location

As discussed in Section 1.2.4, appropriate sensor location is mandatory for successful indirect composition control. The temperature profiles plotted in Figure 5.7 were used to illustrate the use of some of the steady state sensor location criteria suggested in the literature. The profiles were generated by simulating the response to ±5% step changes in distillate flow rate with constant reflux rate and reboiler duty. As discussed in Section 1.2.3 and suggested by Tolliver and McCune (1978), sensors should be located on that tray on which temperatures exhibit maximum symmetrical changes in response to changes of equal magnitude and opposite direction in the distillate to feed ratio.

As mentioned in Section 5.1, the objective for single quality control was control of either product composition. When considering sensor locations it was therefore desirable to select one tray in each of the rectification and stripping sections of the column. Based on the temperature profiles in Figure 5.7 there is no stage in the rectification section on which the magnitude of the

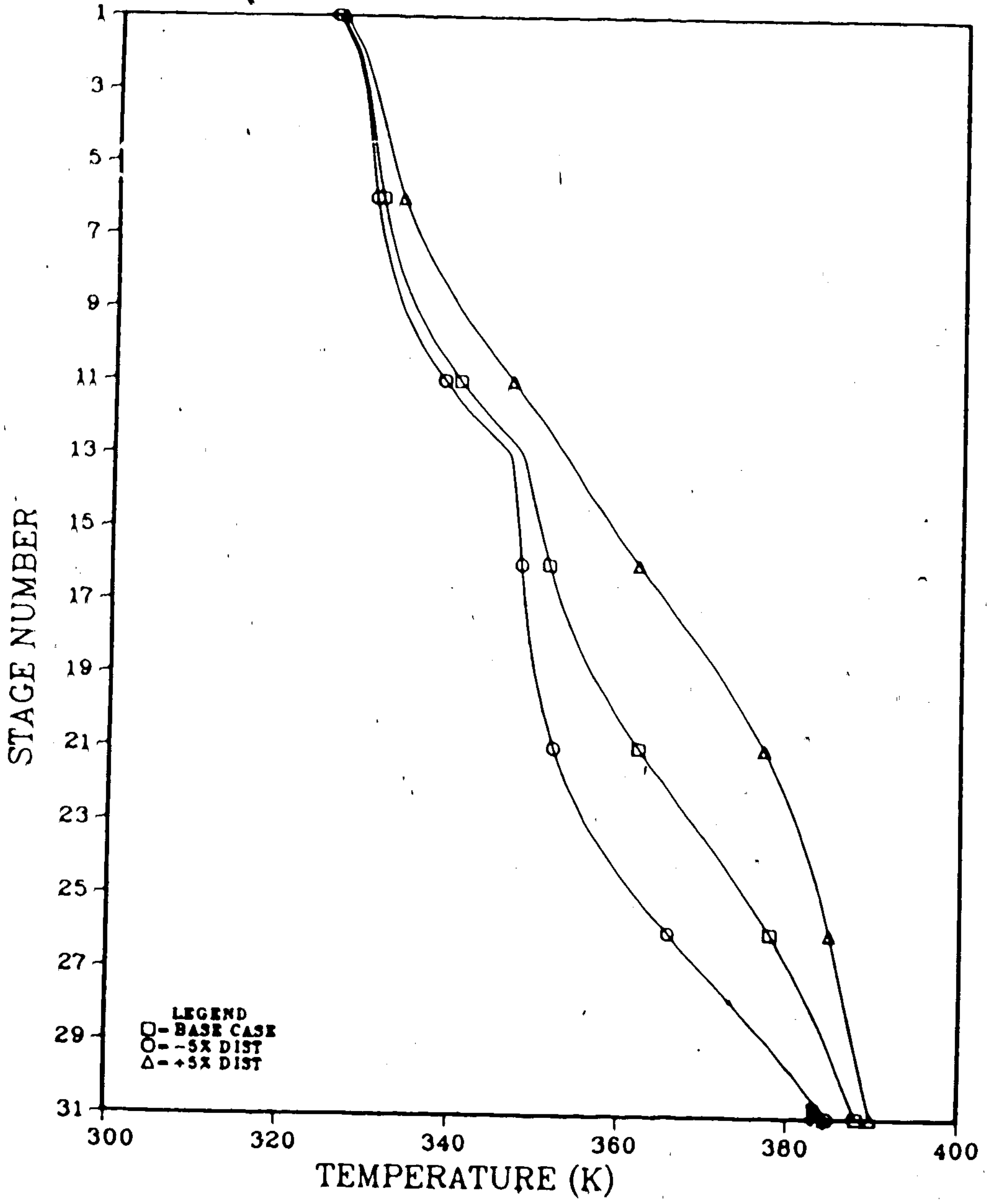


Figure 5.7

TEMPERATURE PROFILES FOR DISTILLATE RATE DISTURBANCE CASES

USED TO DETERMINE TEMPERATURE SENSOR LOCATIONS temperature change after a 5% distillate rate decrease is equal to that after a 5% distillate rate increase. The degree of nonlinearity is smaller for trays higher in the section than for those closer to the feed point. On the other hand, the temperature gradient is smaller at the top of the column than it is closer to the feed tray. As a compromise between the criteria of maximum temperature gradient and maximum symmetrical profile displacement from the base case profile, stage 6 (i. e. the 5th tray numbering from the top of the column) is selected as the sensor location in the rectification section.

Stages below the feed plate were considered for control of the bottom product composition. In the stripping section the temperature profiles after ±5% distillate rate changes are relatively symmetrical. Stage 23 displays almost equal magnitude temperature changes from the base case values in response to disturbances of equal magnitude. The temperature gradient at this stage is also reasonably large. Based on steady state considerations, then, stage 23 appears to be a reasonable tray on which to locate a temperature sensor.

The dynamic responses to feed rate disturbances of the temperatures on the trays flagged as viable sensor locations were studied and are plotted in Figures 5.8 and 5.9 for a 10% feed rate decrease and a 10% feed rate increase respectively. The temperature responses on the two trays adjacent to the potential control trays are also plotted.

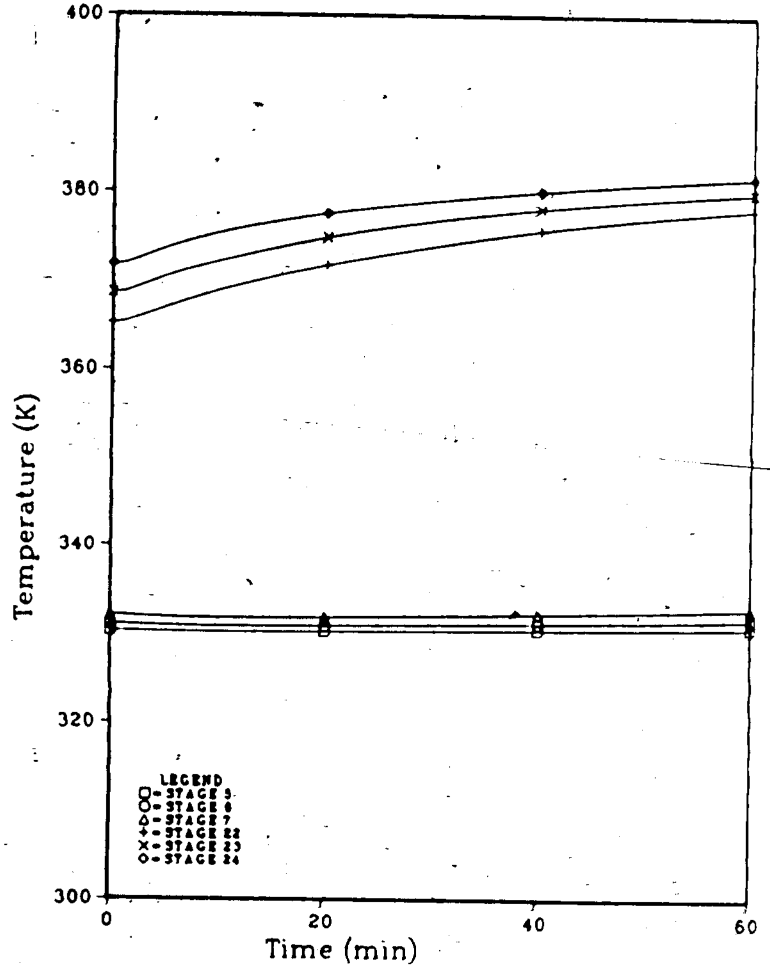


Figure 5.8
POTENTIAL CONTROL TRAY
TEMPERATURE RESPONSES TO A
10% FEED RATE DECREASE

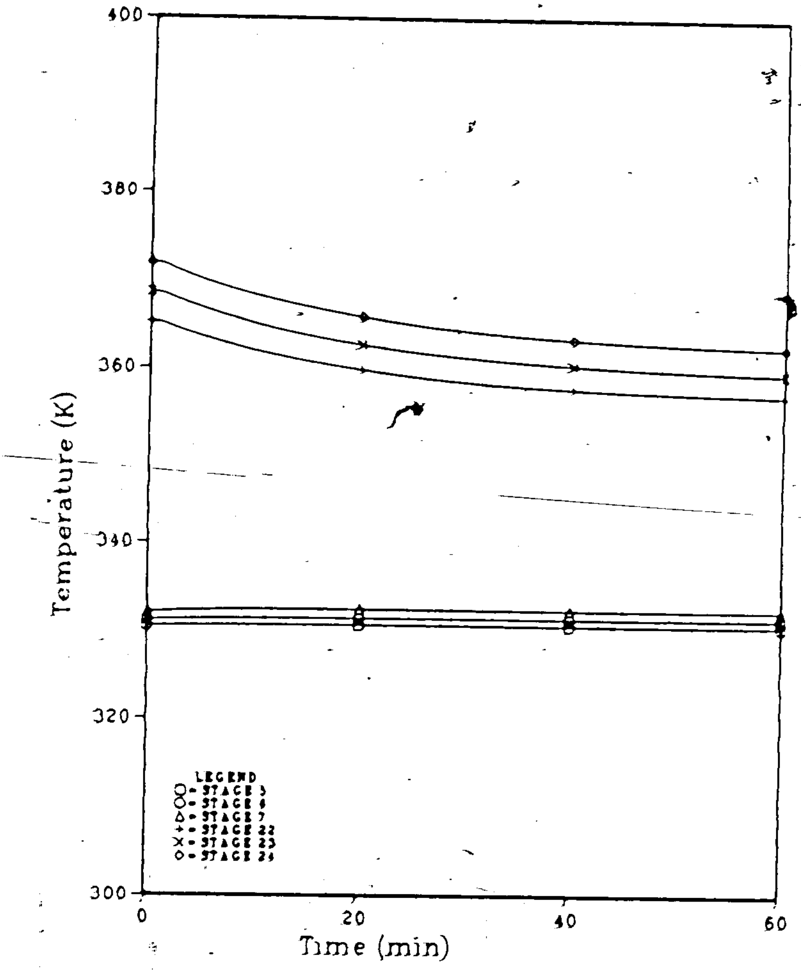


Figure 5.9
POTENTIAL CONTROL TRAY
TEMPERATURE RESPONSES TO A
10% FEED RATE INCREASE

The stage temperatures in the rectification section are quite insensitive to the disturbances. Since the liquid distillate composition has been shown to be very sensitive to feed rate disturbances (cf Chapter 3), the correlation between the rectification stage temperatures and the distillate product composition is unlikely to be strong. Since tray 6 is as responsive as the trays adjacent to it, it still appeared to be the best choice for a rectification section control tray. Control cases based on it should be examined for evidence of the effect of the lack of dynamic responsiveness of the stage temperature on the control performance. The dynamic responses of the temperature on stage 23 to the feed rate increase and decrease are large and fast enough to qualify that stage as the location for a stripping section temperature sensor.

5.3.2 Indirect Single Quality Control

Having selected the locations for temperature sensors as stage 6 for the control of top product composition and stage 23 for control of bottom product composition, design of controllers was required. Control above and below the feed are considered separately.

Indirect Distillate Composition Control

The control strategy used is shown schematically in Figure 5.10. Reflux rate is manipulated to control the temperature on stage 6 and hence the distillate composition. A proportional-integral controller was selected as typical

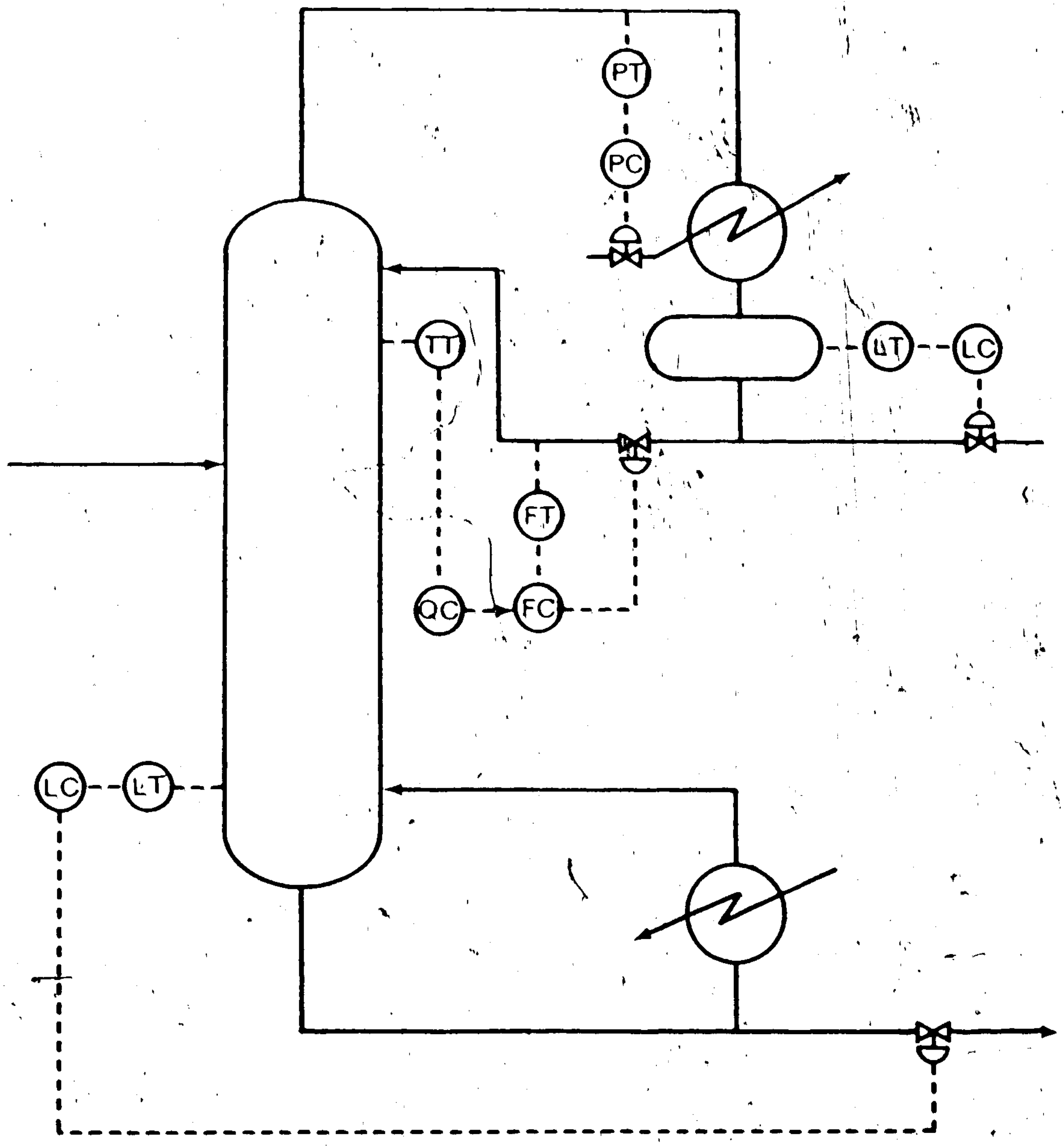


Figure 5.10

SINGLE QUALITY CONTROL SCHEME FOR INDIRECT DISTILLATE COMPOSITION CONTROL for this type of application.

Initial controller settings were calculated using the Cohen and Coon method (Coughanowr and Koppel, 1965) based on open loop dynamic response to changes in reflux rate. The response curves for 10% reflux rate increases and decreases are plotted in Figures 5.11 and 5.12 respectively. Comparing the response of stage 6 temperature in the two plots, it is immediately obvious that the response is highly nonlinear. Since the control loops were to be tuned for feed rate decreases, the response to reflux rate decrease was used to evaluate initial controller settings. Initial controller settings for this and the other single quality control cases are summarized in Table 5.1. Responses of the column variables of interest to a 10% feed rate decrease with indirect control of the distillate composition using the temperature feedback controller with the temperature sensor on stage 6 and with the initial Cohen and Coon controller parameters is shown in Figure 5.13. Limits of ±25% of the steady state reflux rate were imposed. The control is erratic and at best marginally stable. Table 5.1 includes a summary of performance indices for the single quality control cases. The IAE performance index value shown on Figure 5.13 is that based on the integral of absolute deviation of the mole fraction of the heavy key, isobutane, in the distillate stream from the desired value of 0.0042. This is denoted in Table 5.1 as the 'TOP IAE'. The integral of the absolute deviation of stage 6

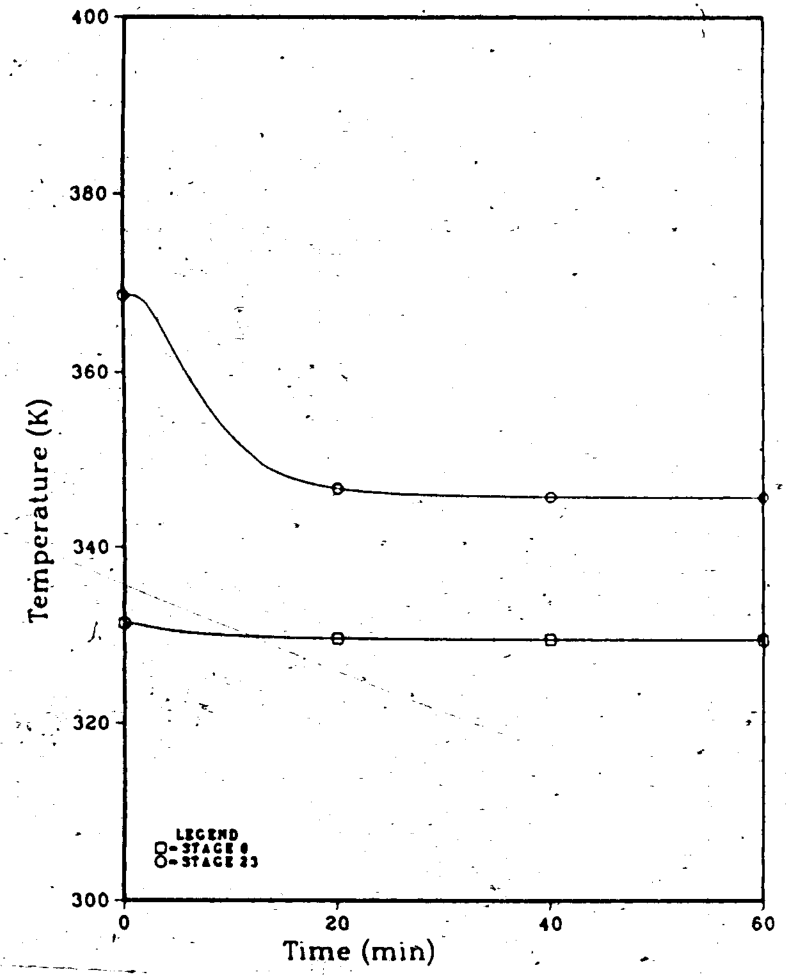


Figure 5.11
CONTROL TRAY TEMPERATURE
RESPONSES TO A 10% REFLUX RATE
INCREASE

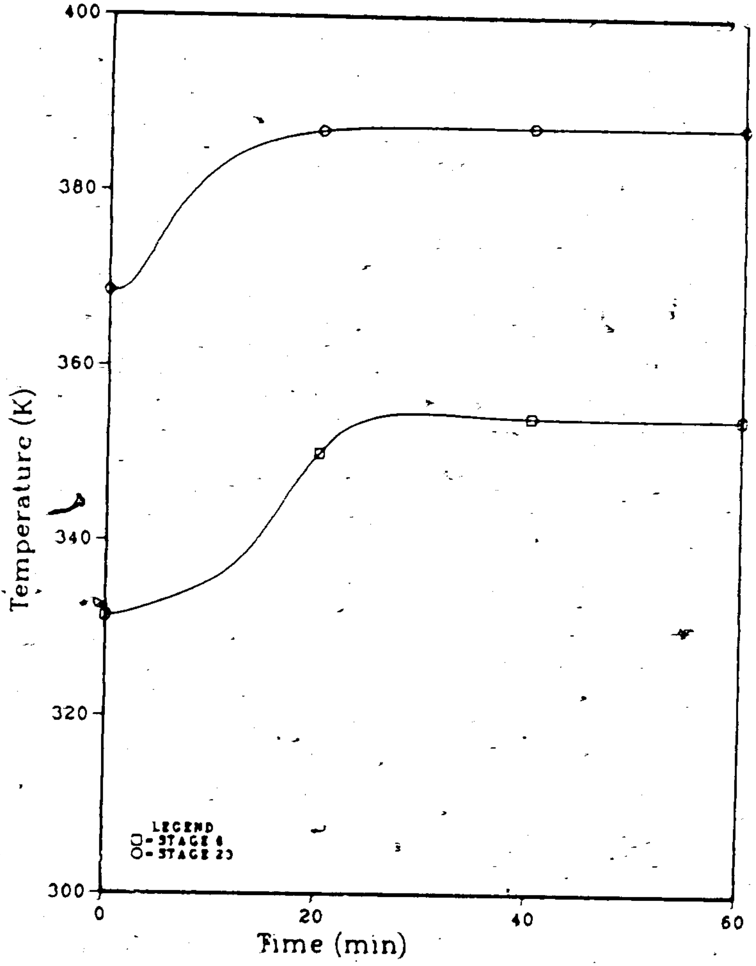
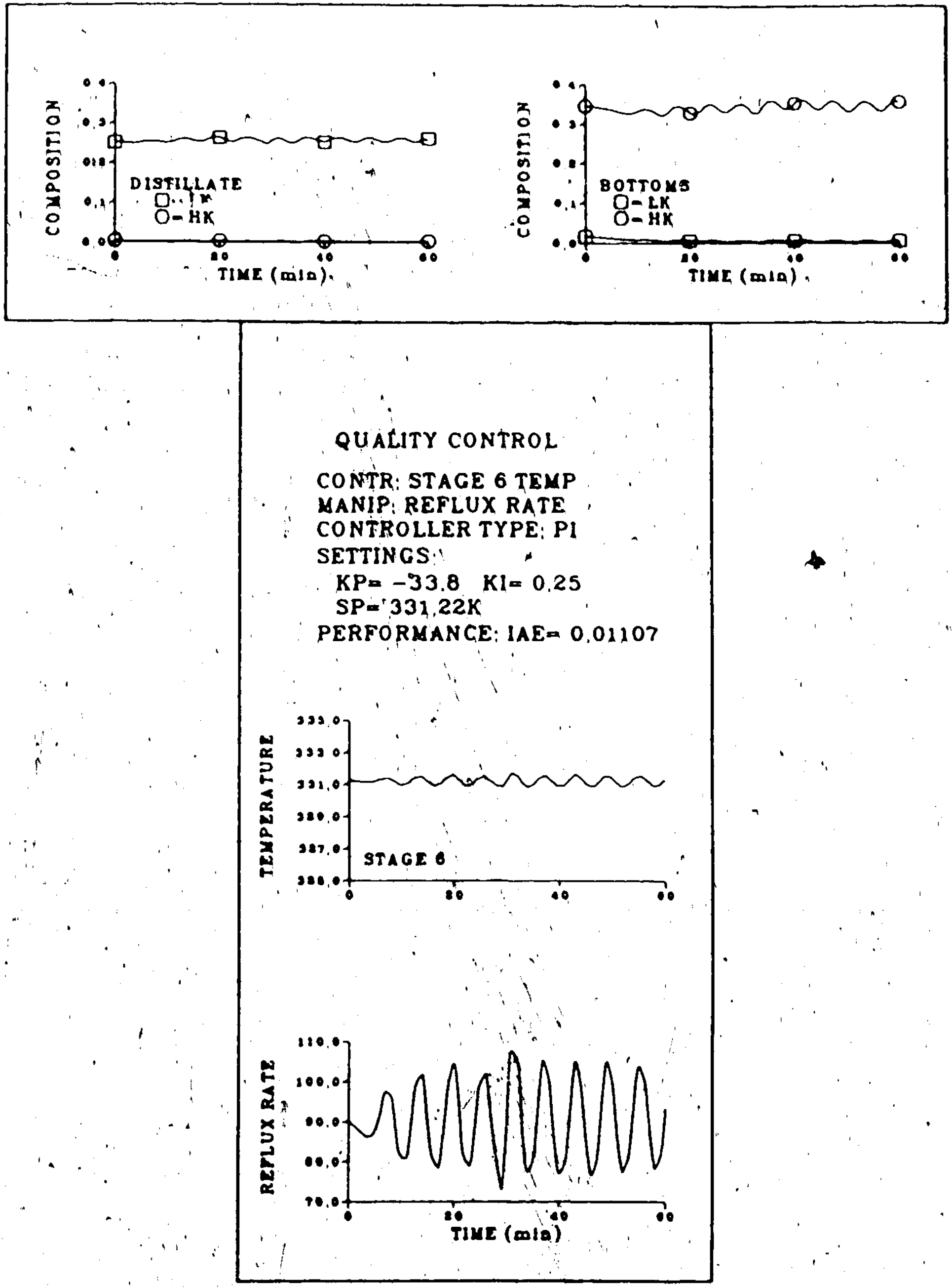


Figure 5.12
CONTROL TRAY TEMPERATURE
RESPONSES TO A 10% REFLUX RATE
DECREASE

Table 5.1

SINGLE QUALITY CONTROLLERS AND CONTROL PERFORMANCE FOR FEED RATE DISTURBANCES

	INITIAL SETTINGS	INITIAL PERFORMANCE	FINAL SETTINGS	PERFORMANCE -10% FEED	PERFORMANCE +10% FEED
INDIRECT CONTROL Objective: Distillate Composition Controlled: Stage 6 Temperature Manipulated: Reflux Rate	K_p= -33.8 K_i= 0.25 SP= 331.22K	LOOP IAE= 14.10 TOP IAE= .01107 BTM IAE= .25035	K_p= -10.0 K_i= 0.10 SP= 331.22K	LOOP IAE= 1.98 TOP IAE= .00988 BTM IAE= .26867	LOOP IAE= 1.05 TOP IAE= .01218 BTM IAE= .58938
INDIRECT CONTROL Objective: Bottoms Composition Controlled: Stage 23 Temperature Manipulated: Reboiler Duty	K_p= 0.024 K_i= 0.52 SP= 368.56K	LOOP IAE= 382.85 TOP IAE= .03739 BTM IAE= .34449	K_p= 0.012 K_i= 0.10 SP= 368.56K	LOOP IAE= 5.54 TOP IAE= .03994 BTM IAE= .04230	LOOP IAE= 5.34 TOP IAE= .06452 BTM IAE= .03081
DIRECT CONTROL Objective: Distillate Composition Controlled: HK in Distillate Manipulated: Reflux Rate	K_p= -221 K_i= 0.10 SP= 0.0042	TOP IAE= .01802 BTM IAE= .29025	K_p= -2000 K_i= 0.10 SP= 0.0042	TOP IAE= .00590 BTM IAE= .29647	TOP IAE= .00268 BTM IAE= .75263
DIRECT CONTROL Objective: Bottoms Composition Controlled: LK in Bottoms Manipulated: Reboiler Duty	K_p= -4.38 K_i= 0.40 SP= 0.0163	TOP IAE= .01492 BTM IAE= .04222	Same as initial		TOP IAE= .06943 BTM IAE= .01792



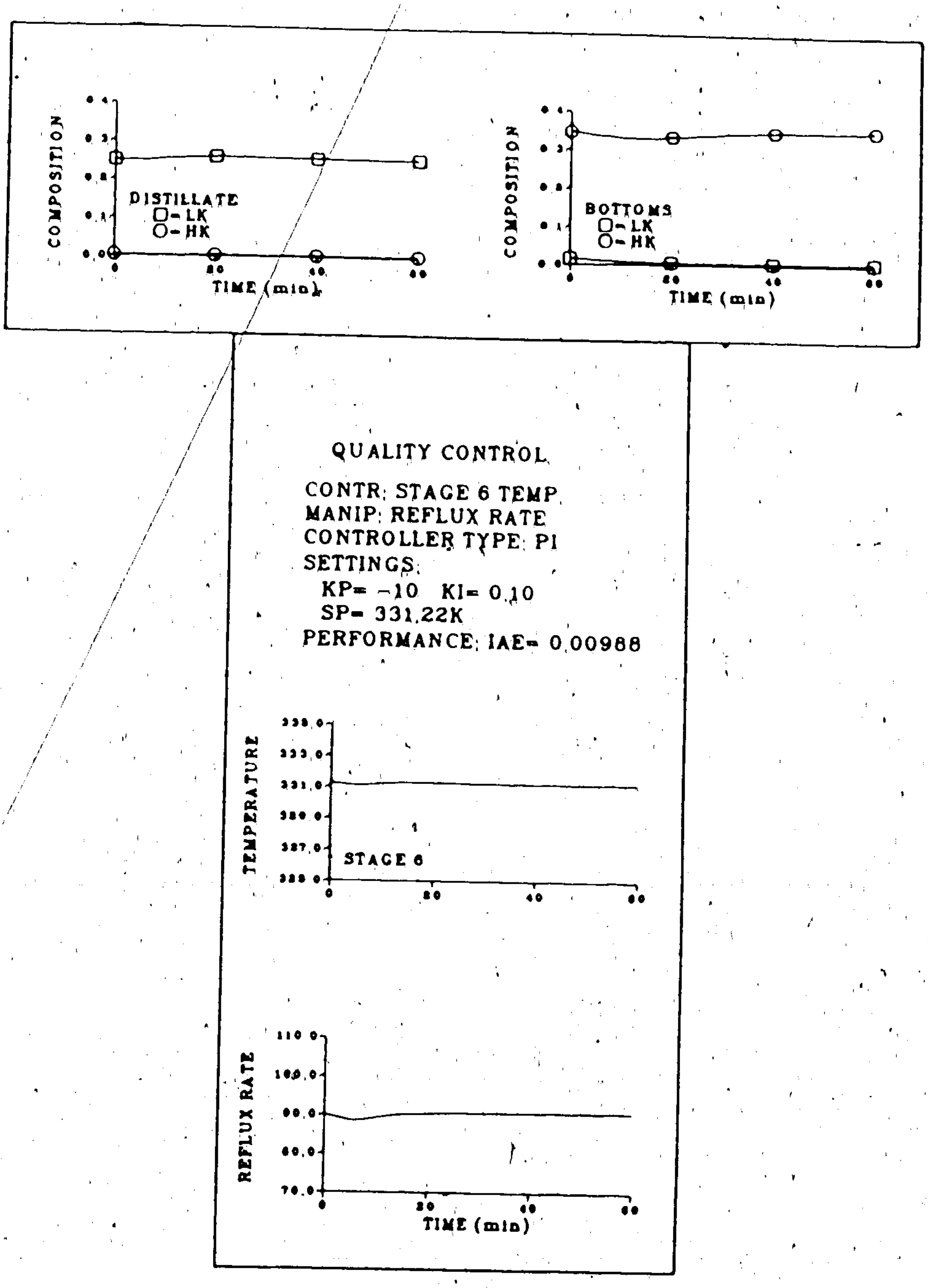
QUALITY CONTROL

CONTR: STAGE 6 TEMP
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -33.8 KI= 0.25
SP= 331.22K
PERFORMANCE: IAE= 0.01107

Figure 5.13

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR INDIRECT SINGLE QUALITY CONTROL OF DISTILLATE COMPOSITION WITH INITIAL CONTROLLER PARAMETERS temperature from its setpoint is listed in Table 5.1 as 'LOOP IAE'. The effect of control of the top product composition on the bottom product composition is calculated as the integral of the absolute error of the mole fraction of the light key, propane, in the bottoms product with respect to the desired value of 0.0163 mole fraction. This performance index is listed in Table 5.1 as 'BTM IAE'. Note that the desired values for product stream impurities are different from those listed in Table 3.1 because the examples in this chapter are simulated using a total condenser.

Tuning of the control loop was performed by trial and error by comparing both the performance indices and dynamic response of the controlled and manipulated variables. The final settings for indirect quality control above the feed stage represents considerable detuning from the Cohen and Coon parameters as the controller gain is about one third of the initial value and the integral constant is reduced by a factor of 2.5. The final settings and the performance indices calculated for the one hour transient period following a 10% decrease in feed rate are noted in Table 5.1. The performance indices for the loop itself and for the top product composition are lower after controller tuning than for the initial controller settings. More impact is seen on the bottom product quality as the control performance above the feed improves. The response trends of the column variables of interest are plotted in Figure 5.14.



QUALITY CONTROL

CONTR: STAGE 6 TEMP
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -10 KI= 0.10
SP= 331.22K
PERFORMANCE: IAE= 0.00988

Figure 5.14

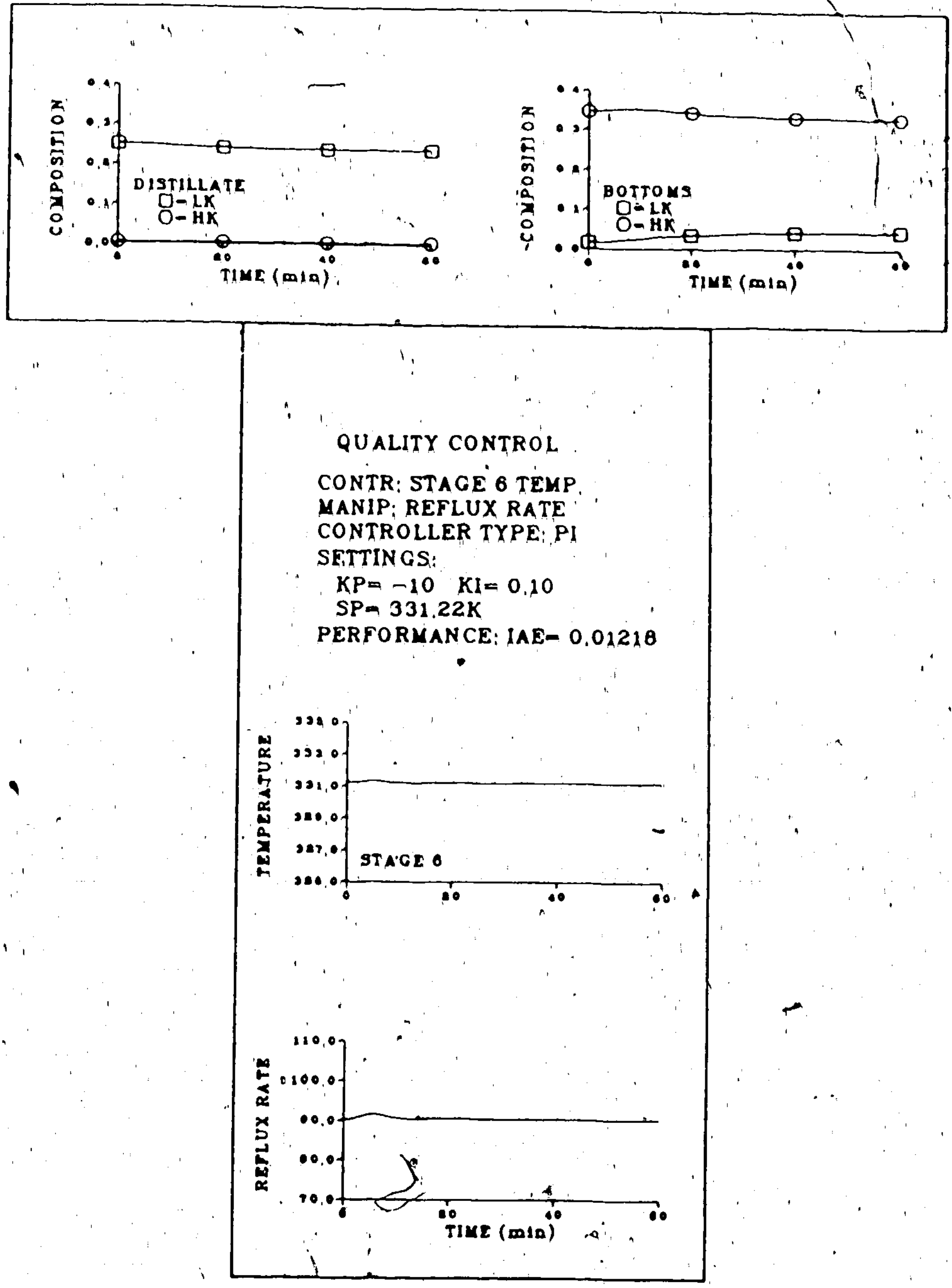
CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR INDIRECT SINGLE QUALITY CONTROL OF DISTILLATE COMPOSITION WITH TUNED CONTROLLER PARAMETERS

The control is sluggish, but the response time seems reasonable. The sluggish characteristic of the control is difficult to avoid because of the fact that stage 6 temperature is insensitive to feed rate disturbances.

An indication of the ability of this controller to handle other disturbances was provided by simulating the closed loop transient following a 10% feed rate increase. The performance indices calculated for this case are also listed in Table 5.1 and Figure 5.15 shows column responses. Since the feed rate increase is less severe than a feed rate decrease, it should be expected that the control performance should be better after a feed rate increase. The loop IAE calculated for the feed rate increase case is less than that calculated for the feed rate decrease case with the same controller settings. The IAE for the top product composition, however, is higher for the feed rate increase than for the feed rate decrease. This observation is another indication that control using stage 6 as the sensor location is less than ideal.

Indirect Bottoms Composition Control

A controller for the indirect control of the bottom product composition by controlling stage 23 temperature was designed following the procedure outlined in the previous paragraphs for indirect control above the feed point. For these cases the temperature feedback controller was assumed to manipulate reboiler duty directly although little additional work would be required to simulate the



QUALITY CONTROL

CONTR: STAGE 6 TEMP.
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= −10 KI= 0.10
SP= 331.22K
PERFORMANCE: IAE= 0.01218

Figure 5.15

CLOSED LOOP RESPONSES TO A 10% FEED RATE INCREASE FOR INDIRECT SINGLE QUALITY CONTROL OF DISTILLATE COMPOSITION WITH TUNED CONTROLLER PARAMETERS manipulation of steam flow rate. Reflux rate was assumed to be on flow control at the base case value of 90 kmol/min.

Initial controller parameters were calculated using the Cohen and Coon method based on the stage 23 temperature responses to ±10% step changes in reboiler duty shown in Figures 5.16 and 5.17 respectively. The stage 23 temperature responses to increases and decreases in reboiler duty are much less nonlinear than was the case for stage 6 temperature responses to increases and decreases in reflux rate. The process time constant, gain and time delay used to calculate the Cohen and Coon parameters were the average of those measured from the responses to the reboiler duty increase and that to the reboiler duty decrease. The settings calculated are listed in Table 5.1. The performance of this controller when the column was subjected to a 10% feed rate decrease is shown in Figure 5.18 with performance indices summarized in Table 5.1. The control performance with the initial parameters is poor and the reboiler duty alternates between the maximum and minimum limits. In subsequent cases the controller was detuned. The final settings listed in Table 5.1 involved reducing the controller gain by a factor of 2 and the integral constant by a factor of 5. The closed loop response trends after a 10% feed rate decrease with the final controller settings are shown in Figure 5.19. The response time achieved in this case is reasonable and the control action is not excessive. The performance indices summarized in Table 5.1

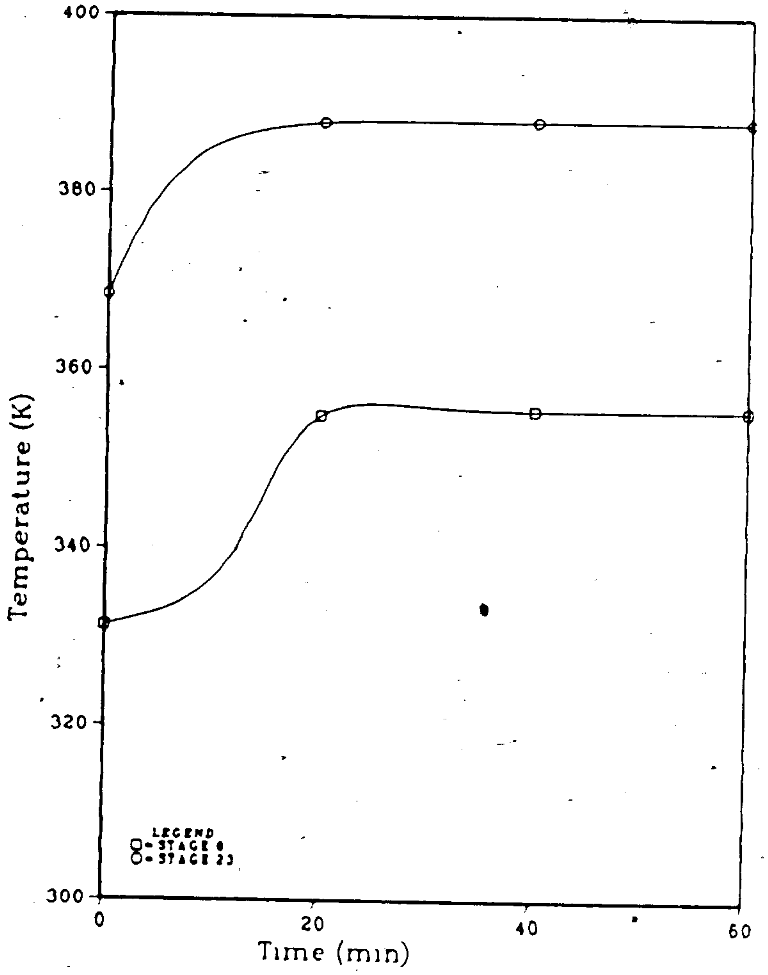


Figure 5.16
CONTROL TRAY TEMPERATURE
RESPONSES TO A 10% INCREASE IN
REBOILER DUTY

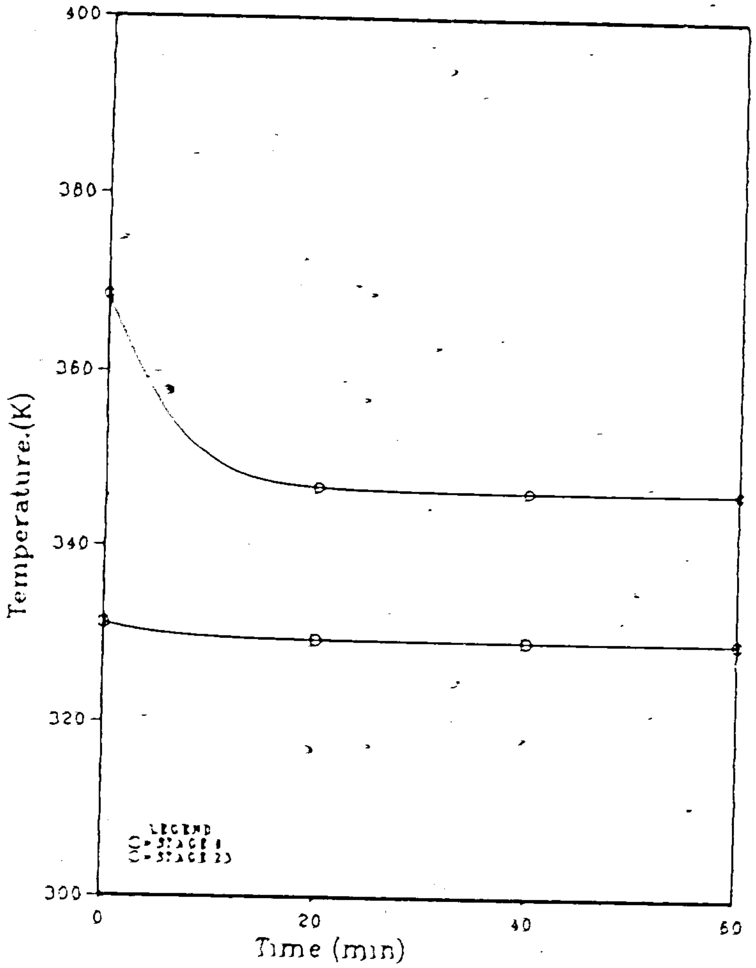
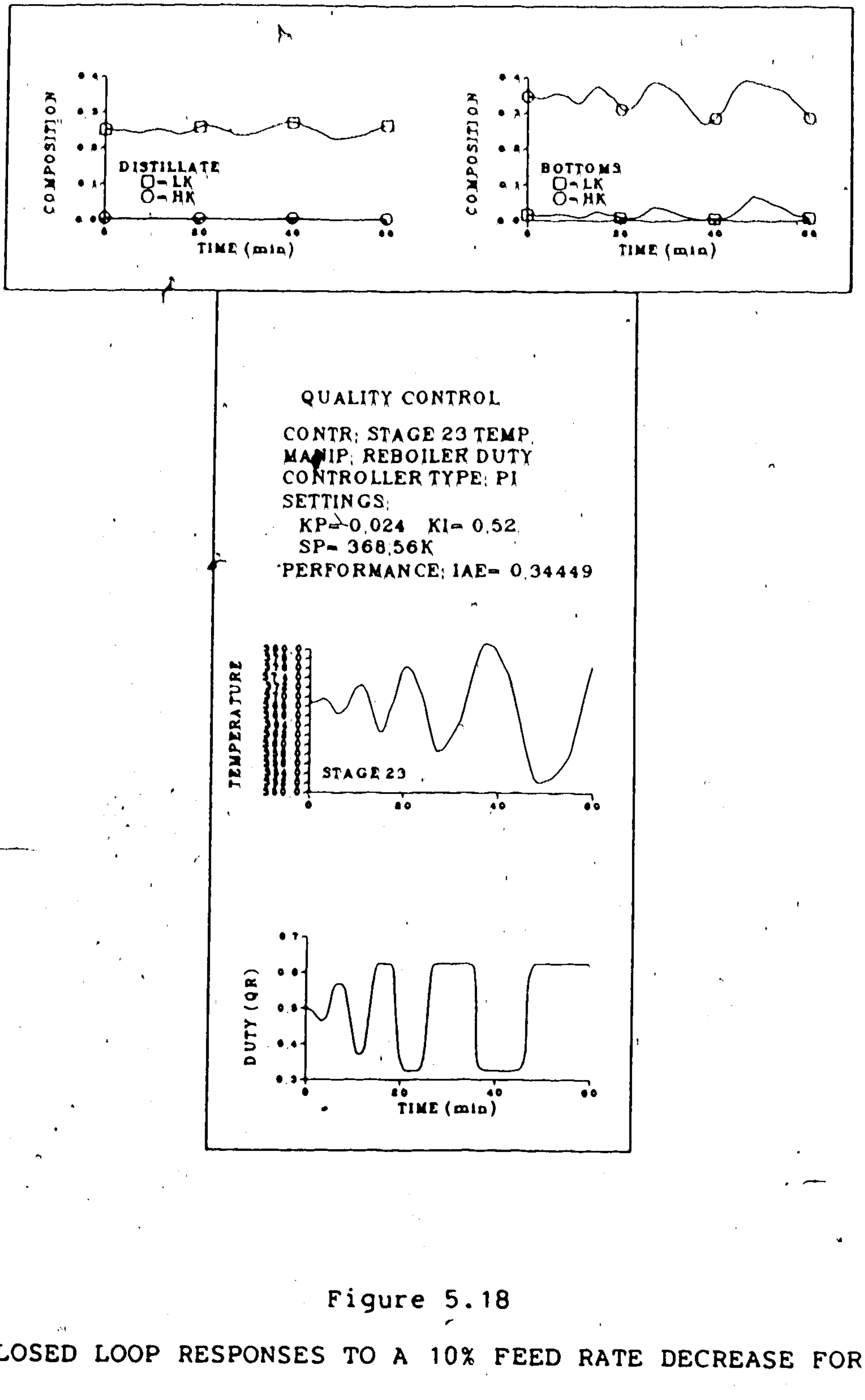


Figure 5.17
CONTROL TRAY TEMPERATURE
RESPONSES TO A 10% DECREASE
REBOILER DUTY

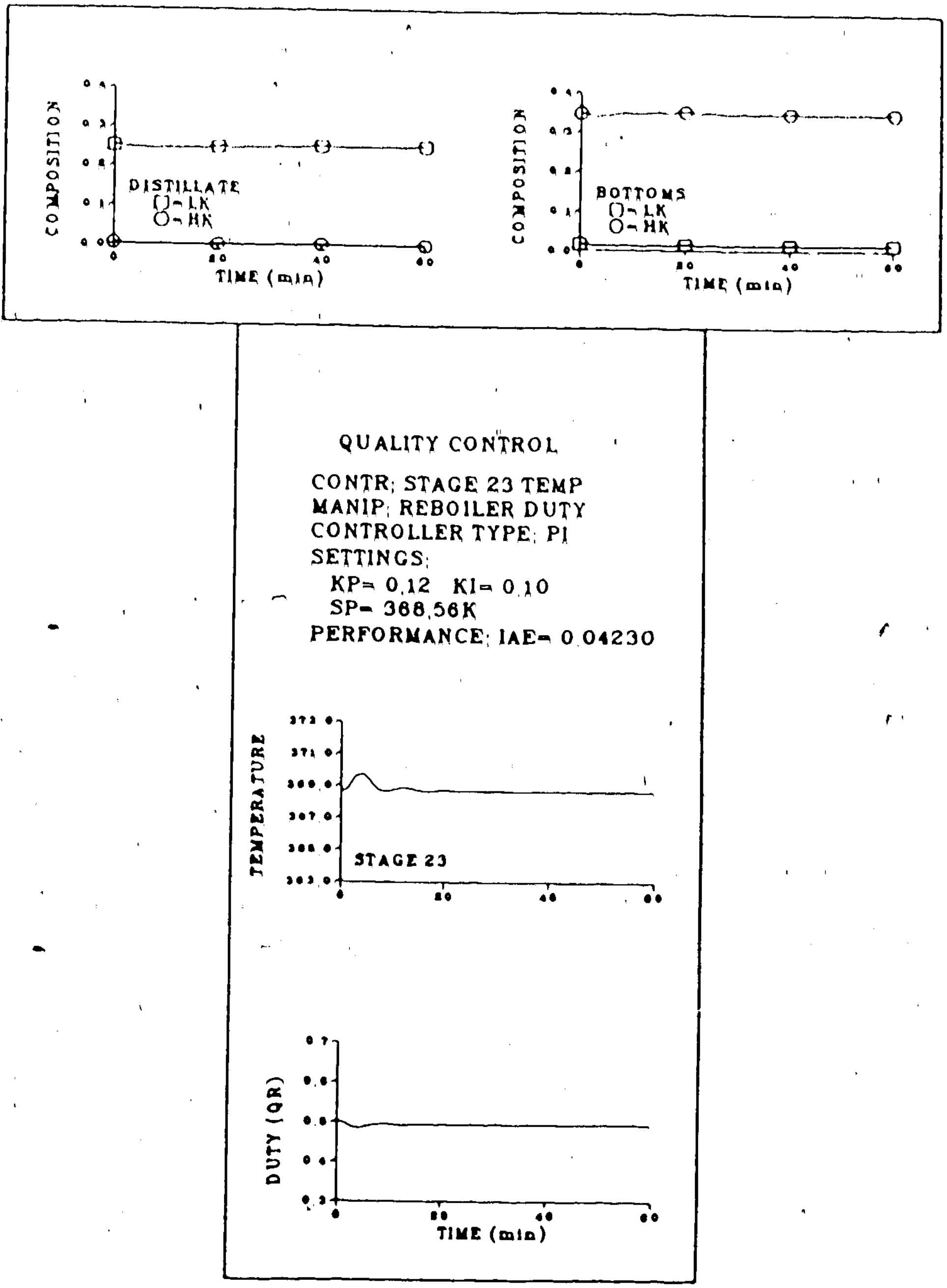


QUALITY CONTROL

CONTR: STAGE 23 TEMP.
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= 0.024 KI= 0.52
SP= 368.56K
PERFORMANCE: IAE= 0.34449

Figure 5.18

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR INDIRECT SINGLE QUALITY CONTROL OF BOTTOMS COMPOSITION WITH INITIAL CONTROLLER PARAMETERS



QUALITY CONTROL

CONTR: STAGE 23 TEMP
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= 0.12 KI= 0.10
SP= 368.56K
PERFORMANCE: IAE= 0.04230

Figure 5.19

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR INDIRECT SINGLE QUALITY CONTROL OF BOTTOMS COMPOSITION WITH TUNED CONTROLLER PARAMETERS indicate significant improvement in both the loop and bottom product IAE measures and only a slight increase in the top product performance index.

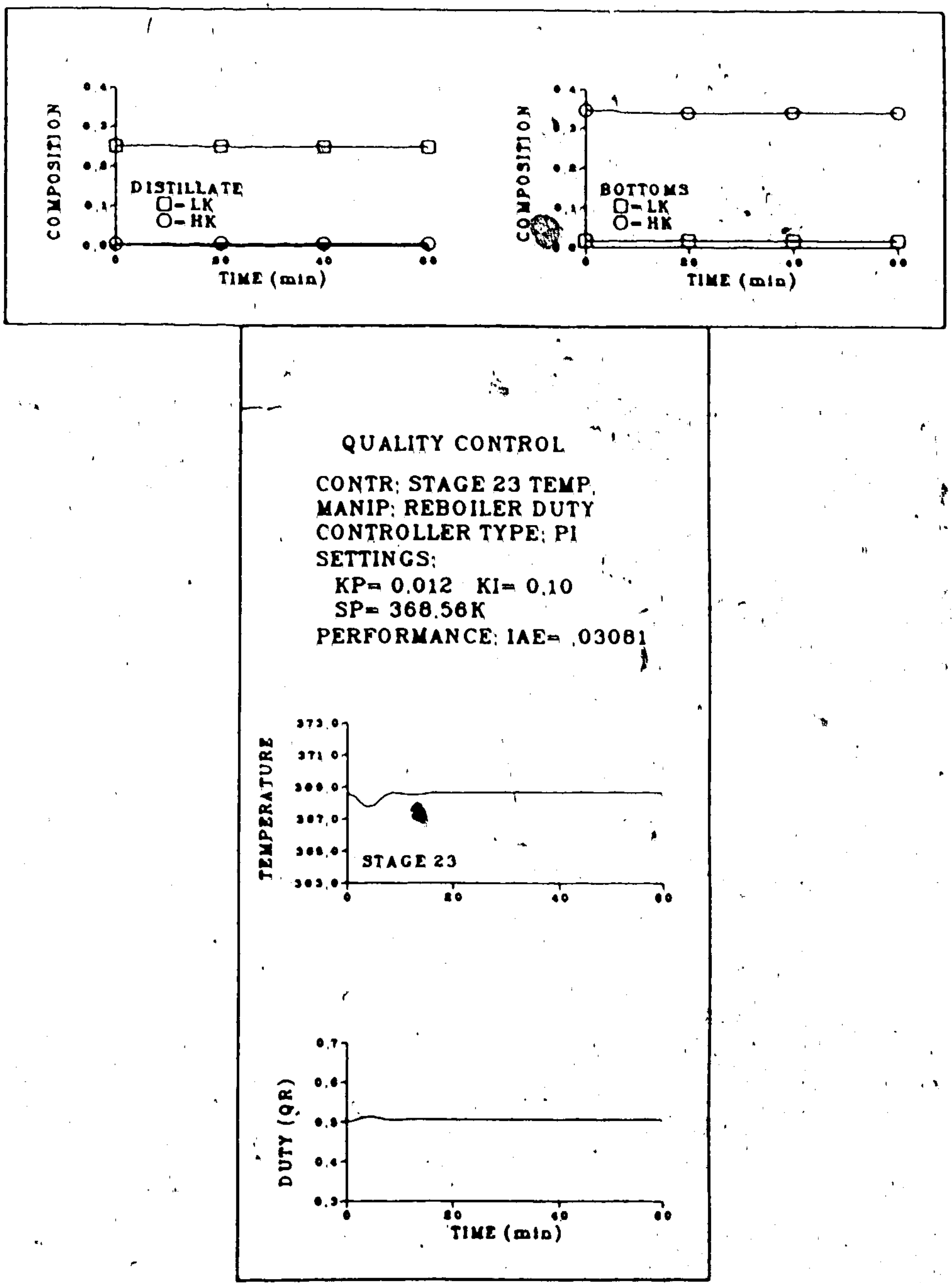
Figure 5.20 shows column response to a 10% increase in feed rate using the final controller settings. For this less severe disturbance the loop and bottom product performance indices are less than those calculated for the feed rate decrease disturbance. This is in contrast with the bad performance of the top product control loop in response to a feed rate increase disturbance, indicating that the more responsive temperature on stage 23 provides a better basis for control than the less sensitive stage 6 temperature, at least with the controller parameters used for these cases.

5.3.3 Direct Single Quality Control

Direct single quality control cases involved the use of the impurity mole fraction in the product stream of interest as the controlled variable. A sketch of the control scheme is shown for direct control of the top product composition in Figure 5.21. For these initial cases no measurement delay was assumed. Top and bottom product quality control are considered separately.

Direct Distillate Composition Control

Cohen and Coon initial controller parameters were evaluated based on the response of the mole fraction of isobutane, the heavy key component, in the distillate stream



QUALITY CONTROL

CONTR: STAGE 23 TEMP.
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= 0.012 KI= 0.10
SP= 368.56K
PERFORMANCE: IAE= .03081

Figure 5.20

CLOSED LOOP RESPONSES TO A 10% FEED RATE INCREASE FOR INDIRECT SINGLE QUALITY CONTROL OF BOTTOMS COMPOSITION WITH TUNED CONTROLLER PARAMETERS

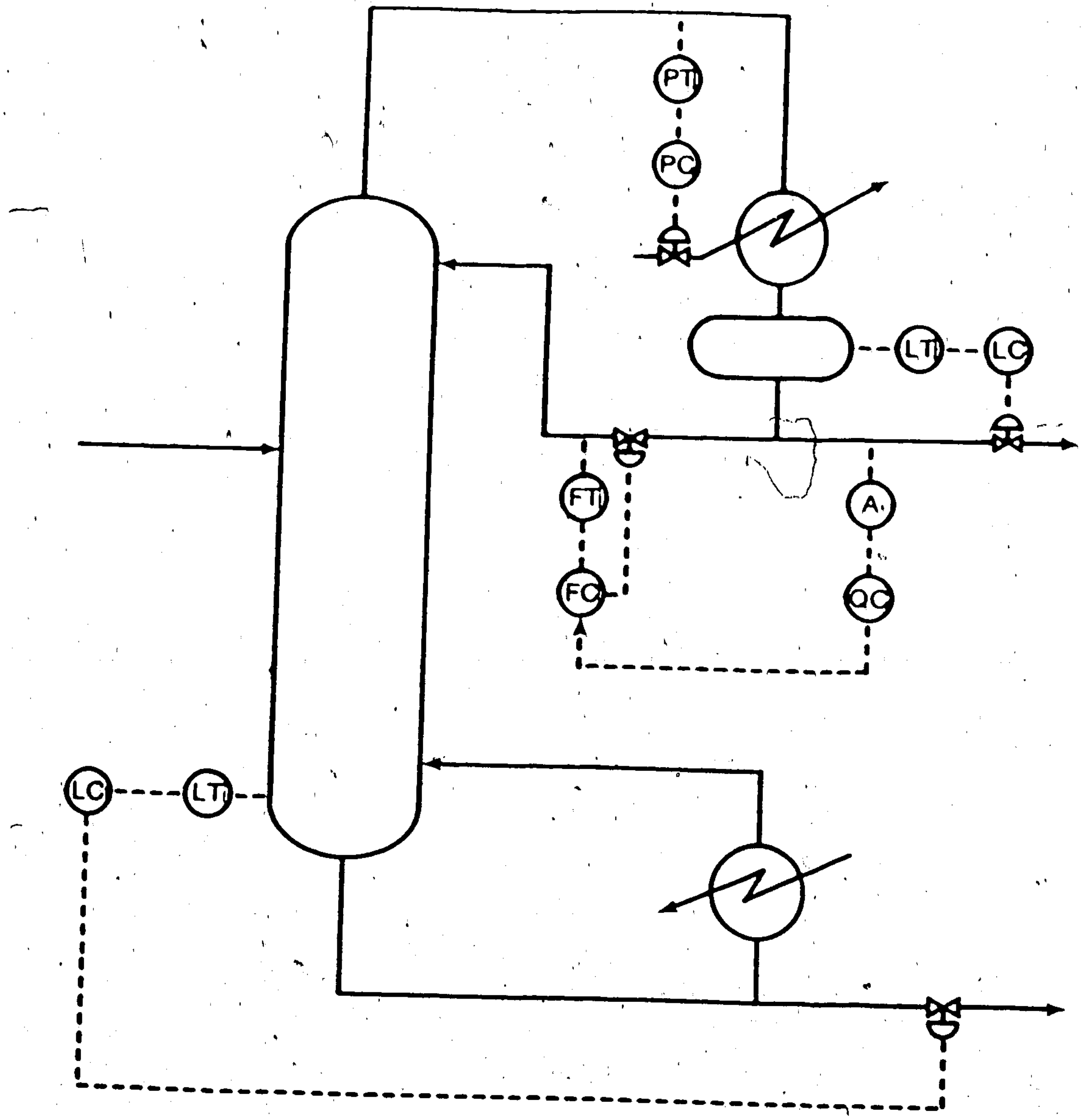
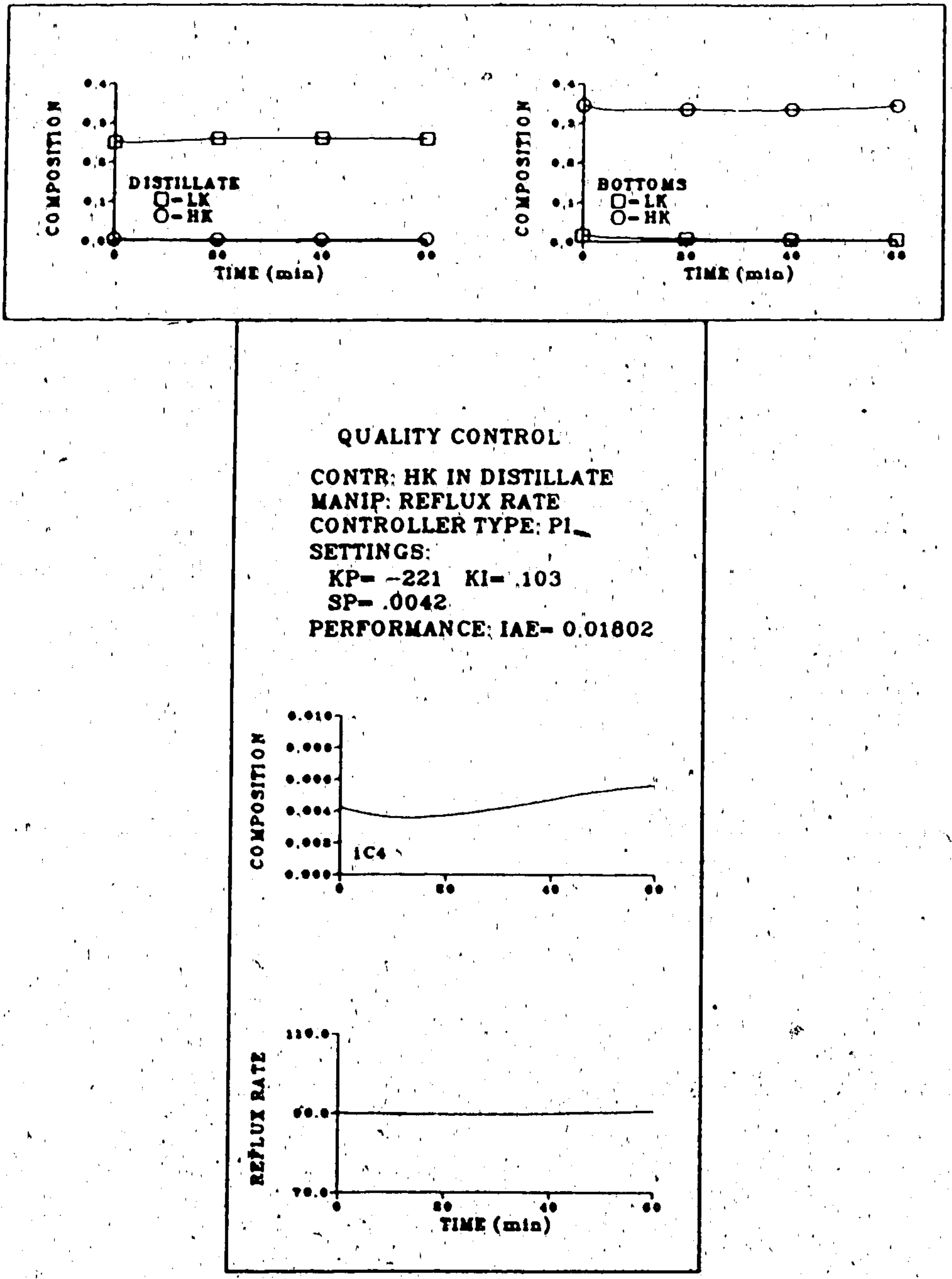


Figure 5.21

SINGLE QUALITY CONTROL SCHEME FOR DIRECT DISTILLATE COMPOSITION CONTROL to increases and decreases in reflux rate. Since the two responses yielded considerably different process model parameters, those based on a reflux rate decrease were used to calculate controller parameters. The initial settings calculated are listed in Table 5.1. Testing this controller with a 10% feed rate decrease led to the responses shown in Figure 5.22. Control is stable, but very slow. As can be seen in Table 5.1, the control performance for direct single quality control of the distillate composition using initial parameters is not as good as that obtained using the initial parameters for indirect quality control of the distillate composition. Considerable improvement was obtained by increasing the controller gain almost tenfold. The performance indices listed in Table 5.1 show a decrease in the top product composition IAE accompanied by a slight increase in the index for the bottom product composition. The column response to a 10% feed rate decrease using the tuned controller is shown in Figure 5.23. The response time is better than was the case with the initial settings. Also, as noted by comparing the performance indices in Table 5.1, the control of both product compositions is better with direct single quality control than with indirect single quality control. However, since neither controller is "optimally" tuned, this observation should not serve as the basis for any broad generalizations.

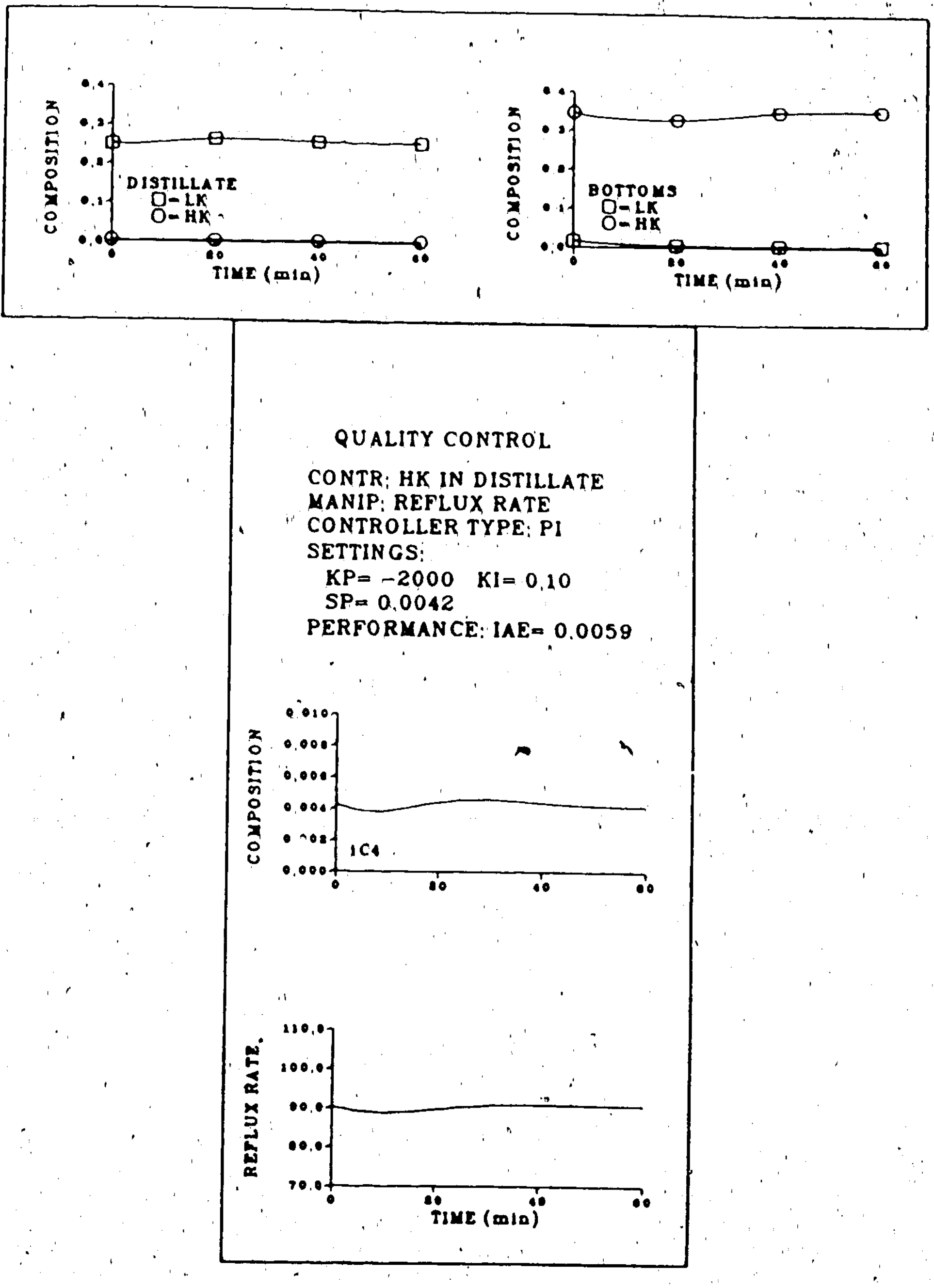
The column response when the system was subjected to a 10% feed rate increase is shown in Figure 5.24 with


QUALITY CONTROL

CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -221 KI= .103
SP= .0042
PERFORMANCE: IAE= 0.01802

Figure 5.22

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR DIRECT SINGLE QUALITY CONTROL OF DISTILLATE COMPOSITION WITH INITIAL CONTROLLER PARAMETERS



QUALITY CONTROL

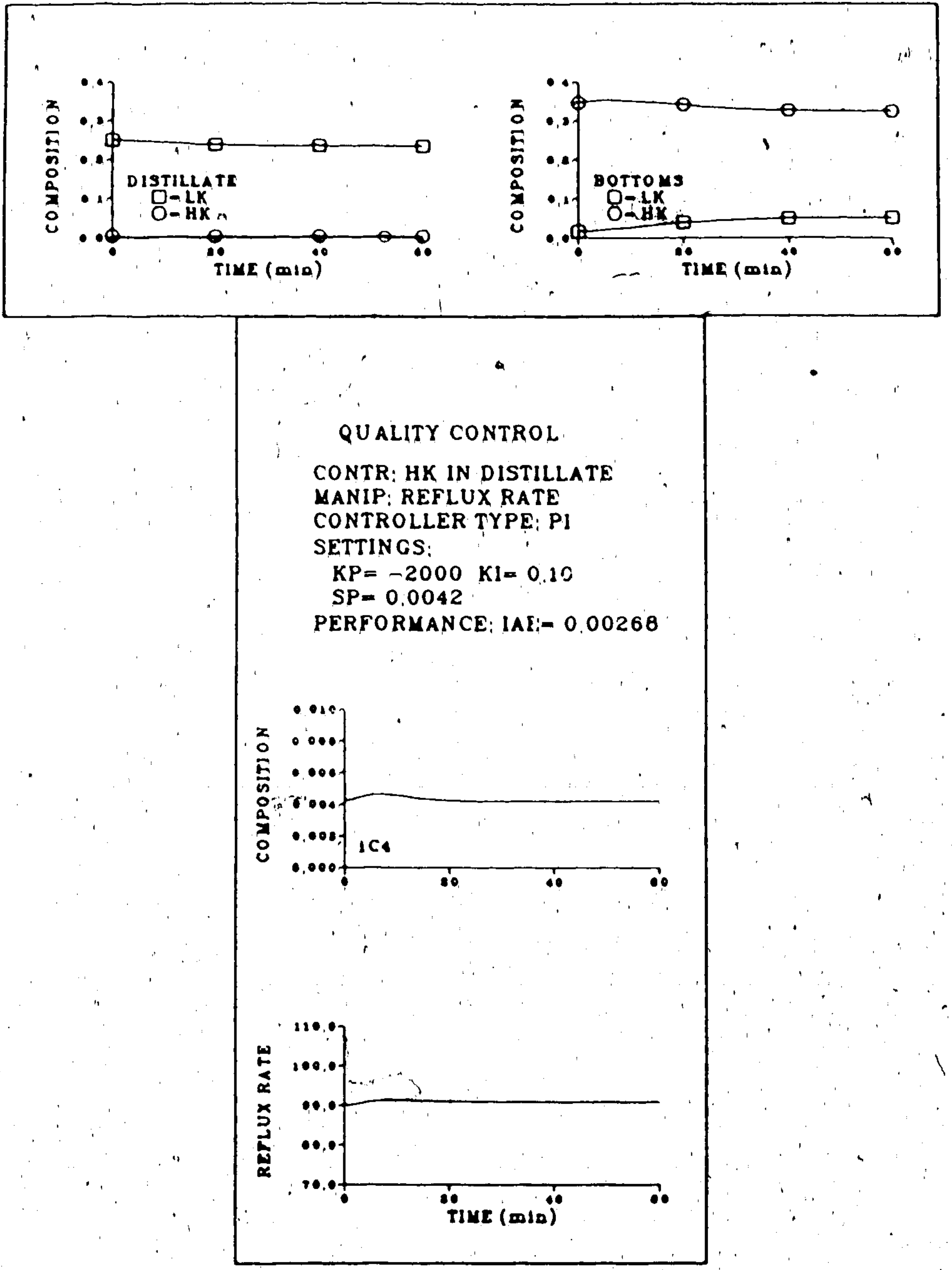
CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -2000 KI= 0.10
SP= 0.0042
PERFORMANCE: IAE= 0.0059

Figure 5.23

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR DIRECT SINGLE QUALITY CONTROL OF DISTILLATE COMPOSITION WITH TUNED CONTROLLER PARAMETERS performance indices shown in Table 5.1. The direct composition controller provided better control for the feed rate increase case than for the corresponding feed rate decrease case, whereas using the indirect controller for a feed rate increase case resulted in top product composition control behaviour that was not as satisfactory as that obtained for the decrease in feed rate. The indirect quality controller does have an advantage over the direct quality controller as seen by comparing the IAE values calculated for the uncontrolled bottoms product composition in each case. Since the indirect quality control case results in sloppy control of the distillate product composition, there are fewer interaction effects on the bottoms product. The bottoms product quality is therefore not perturbed from its initial value, so that the IAE measure calculated for the indirect case is smaller than that calculated for the direct quality control case. Again, this may be a function of the controller tuning rather than of the type of control.

Direct Bottom Product Composition Control

Initial Cohen and Coon parameters for control of the bottom product composition based on measurement of the mole fraction of propane, the light key component, in the bottoms were calculated based on response of the impurity mole fraction to decreases in reboiler duty. The component mole fraction responses to increases and decreases in the manipulated variable were quite different so the response to



QUALITY CONTROL

CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -2000 KI= 0.10
SP= 0.0042
PERFORMANCE: IAE= 0.00268

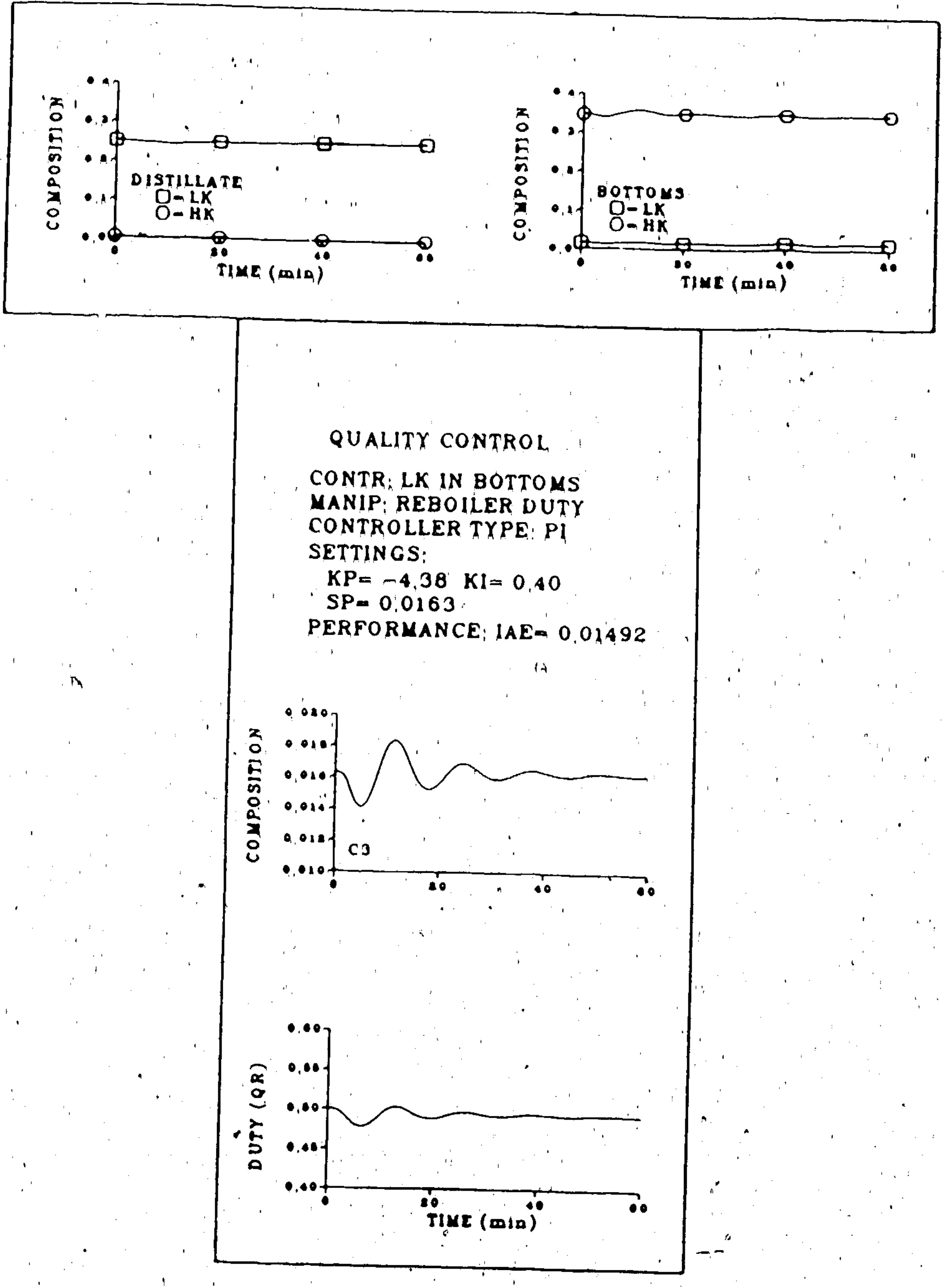
Figure 5.24

CLOSED LOOP RESPONSES TO A 10% FEED RATE INCREASE FOR DIRECT SINGLE QUALITY CONTROL OF DISTILLATE COMPOSITION WITH TUNED CONTROLLER PARAMETERS a decrease in reboiler duty was used to calculate Cohen-Coon settings. The initial settings are given in Table 5.1. Figure 5.25 shows system response to a 10% feed rate decrease using the direct quality controller with initial settings. The response and controller performance were considered satisfactory so no further tuning was performed. The performance indices for both the top and bottom product compositions were better with the initial direct quality control settings than with the final corresponding indirect quality control settings. The controlled response to a 10% feed rate increase is shown in Figure 5.26. The performance is again better than that obtained with the indirect bottom composition controller, although there is a slight deterioration in top product composition control performance compared with that calculated using stage 23 temperature for control.

5.4 Dual Quality Control

5.4.1 Dual Quality Controller Design and Performance

Ideally, simultaneous control of both product compositions is desired. A dual indirect quality control scheme is shown in Figure 5.27 with the corresponding direct quality control scheme shown in Figure 5.28. For the simulation work discussed here the first pass at designing controllers suitable for dual product composition control was the combination of the single loop controllers discussed

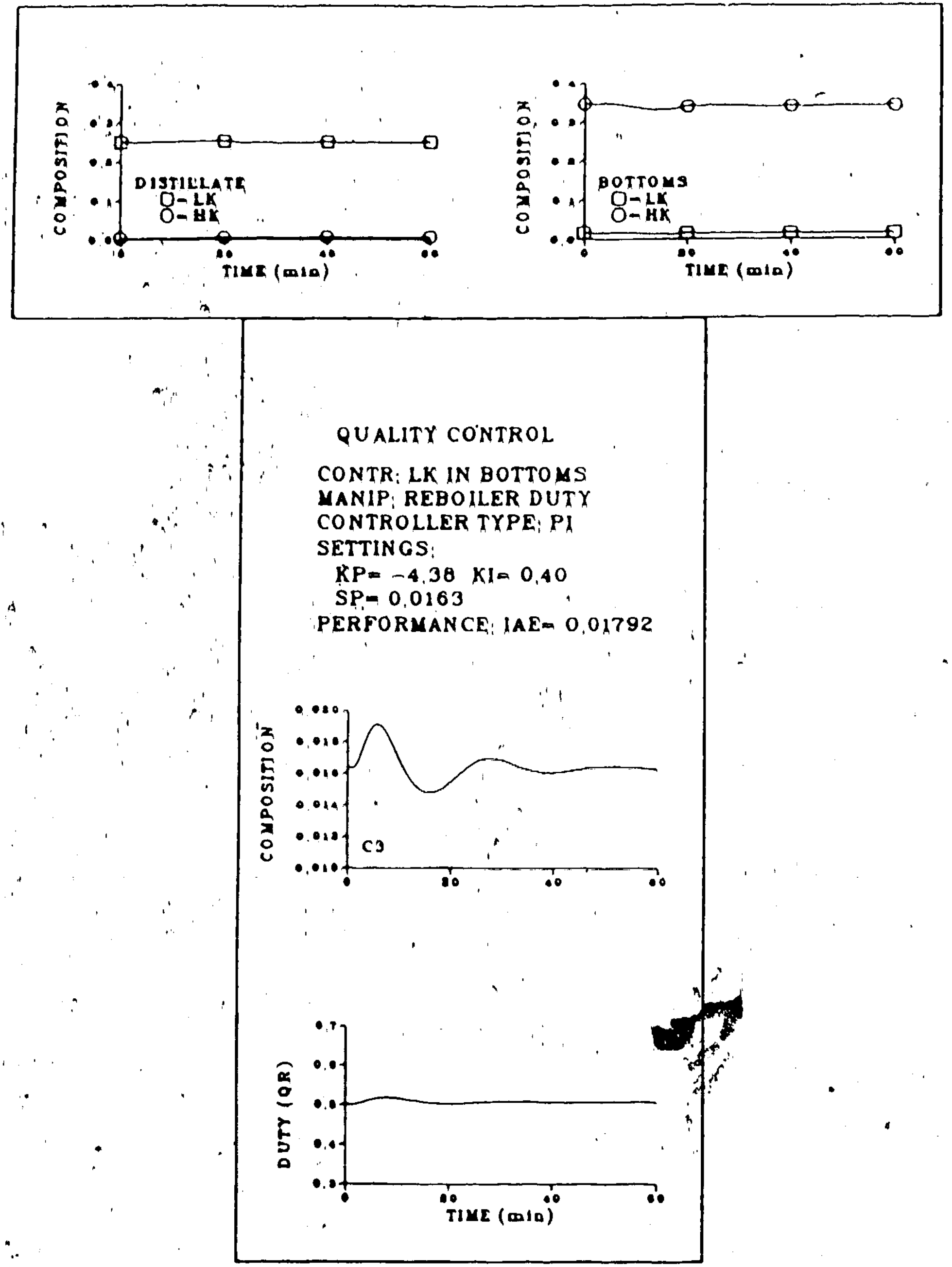


QUALITY CONTROL

CONTR: LK IN BOTTOMS
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= -4.38 KI= 0.40
SP= 0.0163
PERFORMANCE: IAE= 0.01492

Figure 5.25

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR DIRECT SINGLE QUALITY CONTROL OF BOTTOMS COMPOSITION WITH INITIAL CONTROLLER PARAMETERS



QUALITY CONTROL

CONTR: LK IN BOTTOMS
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= -4.38 KI= 0.40
SP= 0.0163
PERFORMANCE: IAE= 0.01792

Figure 5.26

CLOSED LOOP RESPONSES TO A 10% FEED RATE INCREASE FOR DIRECT SINGLE-QUALITY CONTROL OF BOTTOMS COMPOSITION WITH INITIAL CONTROLLER PARAMETERS

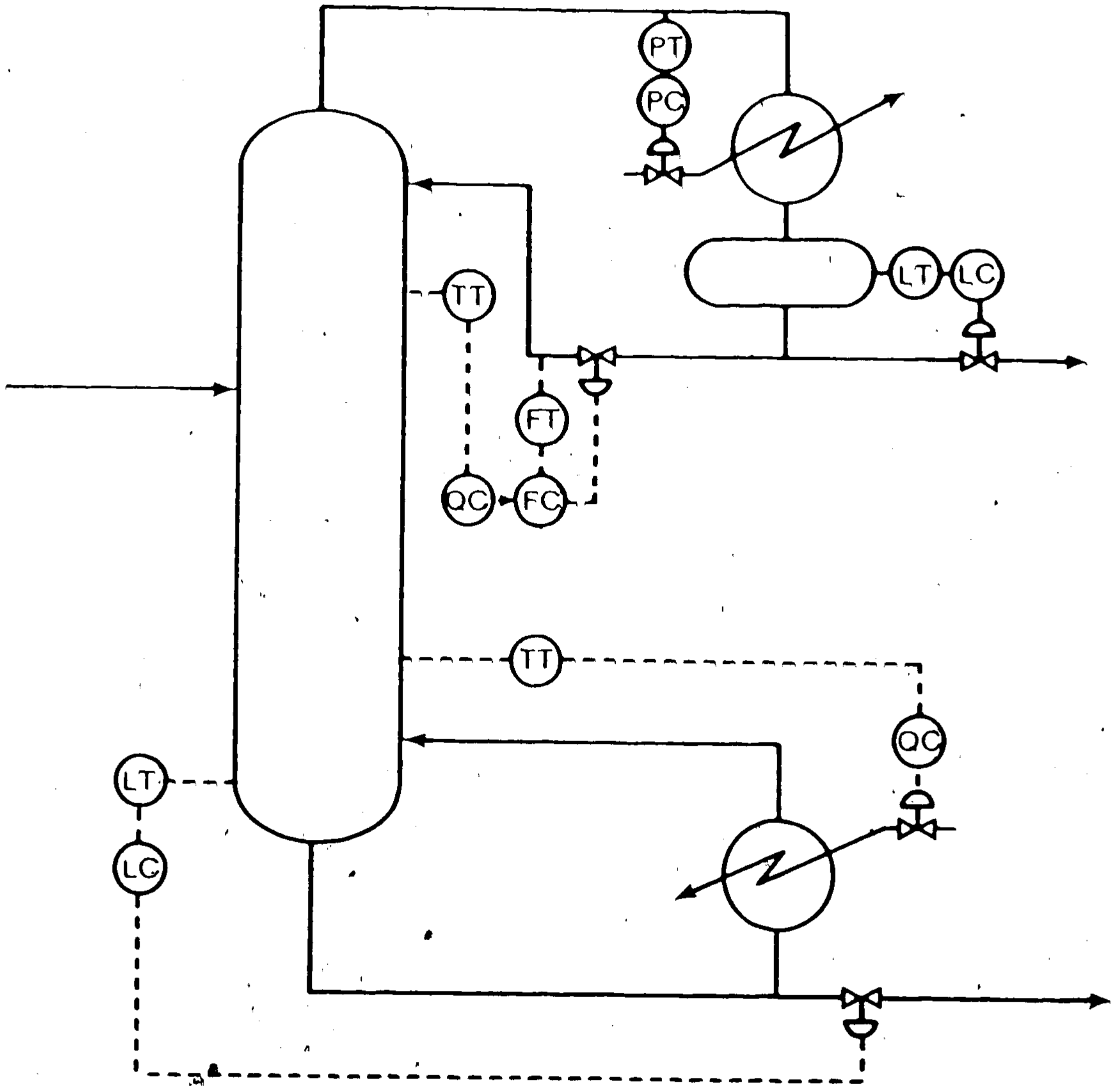


Figure 5.27

INDIRECT DUAL QUALITY CONTROL SCHEME

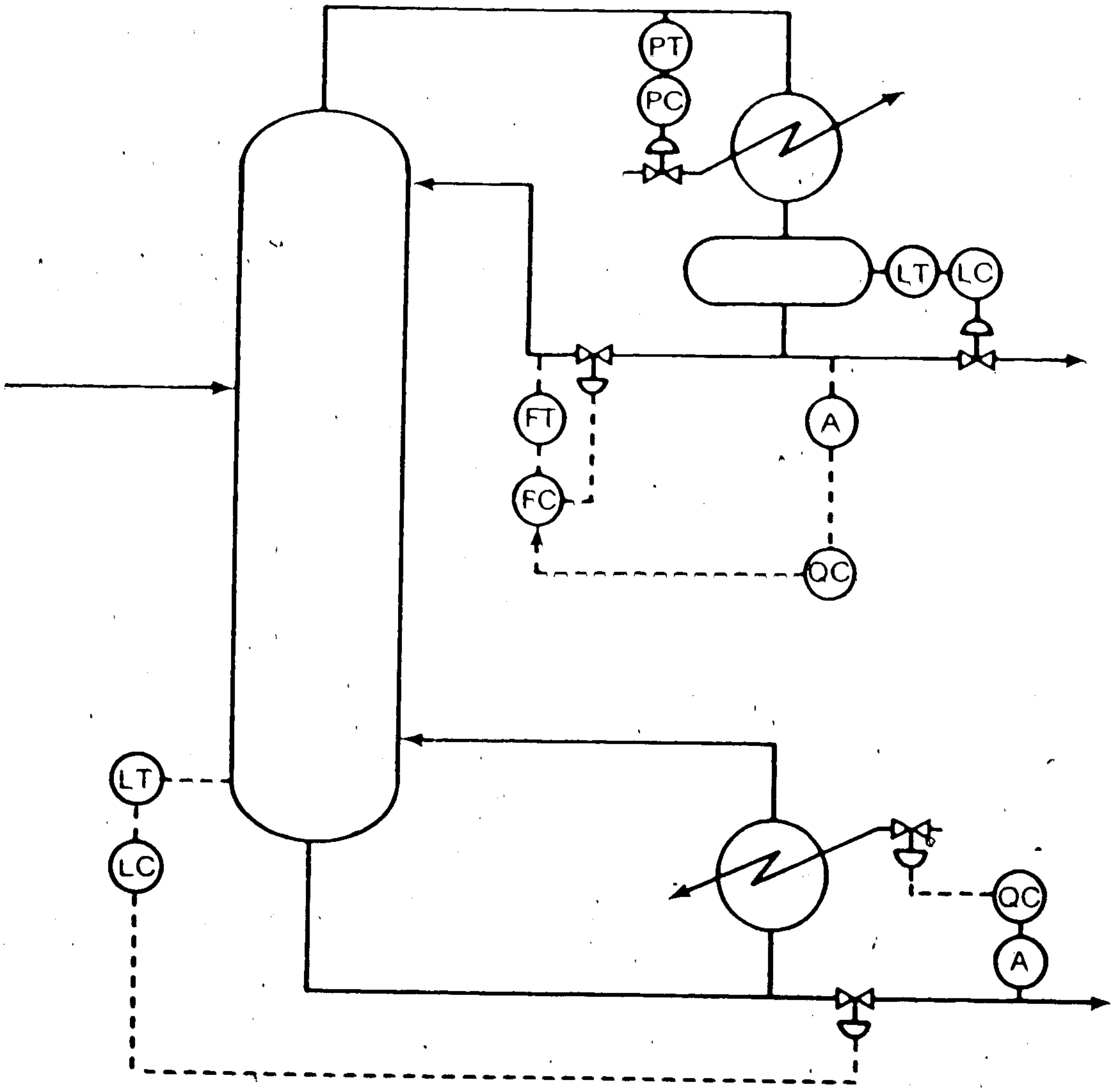


Figure 5.28

DIRECT DUAL QUALITY CONTROL SCHEME

in Section 5.3.

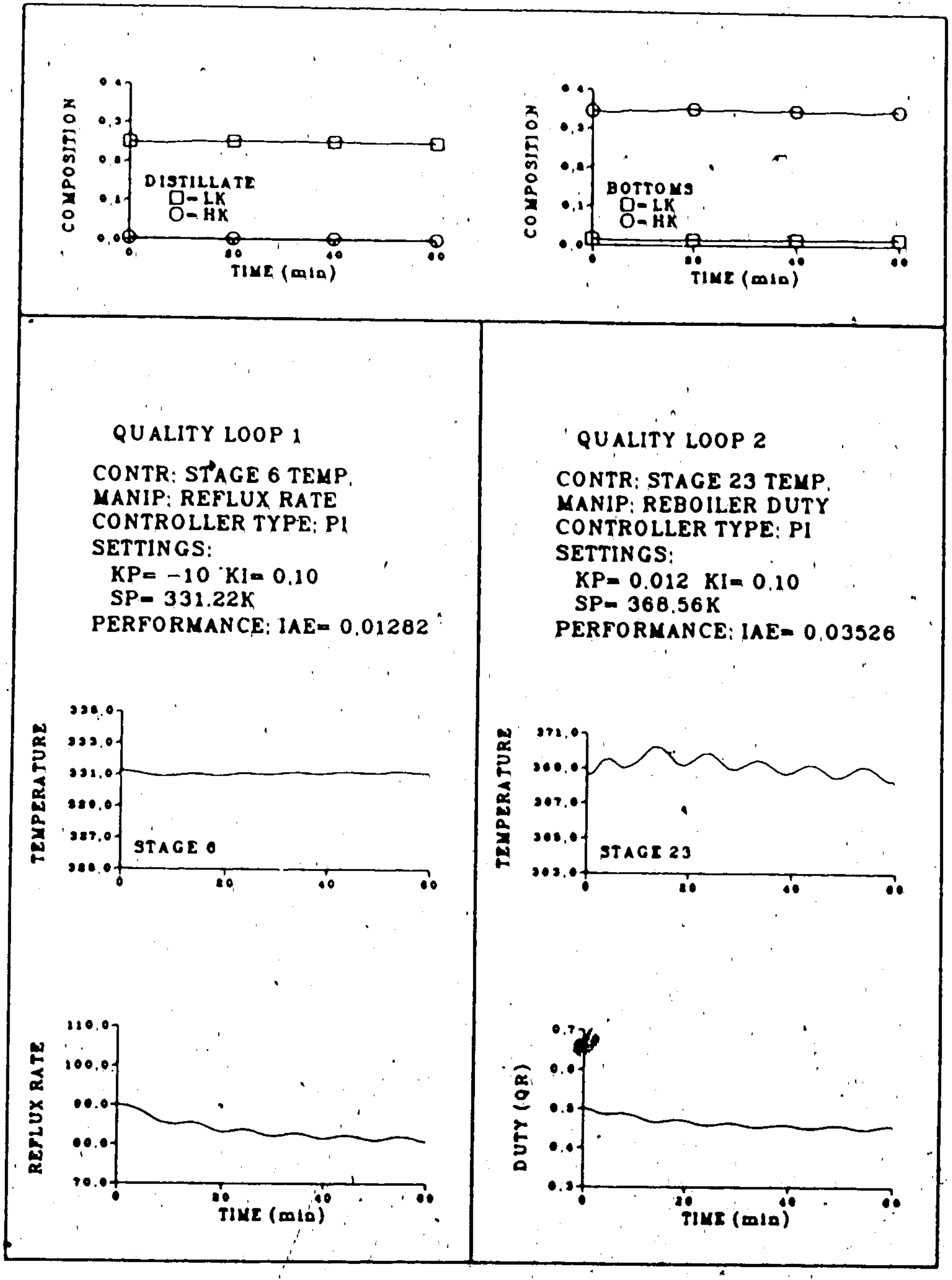
System responses for indirect dual quality control during the transient period after a 10% feed rate decrease are shown in Figure 5.29. The performance index for the top product composition control is almost 25% higher than it was for the single loop case. On the other hand, the performance index for the bottom product composition control is lower than it was in the single loop case by about 17%. The response of stage 23 temperature is somewhat oscillatory and, more importantly, the reboiler duty and reflux rate vary in a manner which may or may not be acceptable depending on other demands on the steam supply and on the system requirements downstream of the column. Further tuning was not attempted since the control was stable and performance reasonable for the purposes of this study.

Combination of the single loop direct quality controllers resulted in the responses to a 10% feed rate decrease shown in Figure 5.30. The response is reasonable but a further tuning case was attempted because the bottoms composition control loop used the original Cohen and Coon parameters calculated for single quality control, so it seemed likely some improvement would be possible. Detuning this controller led to slightly better performance as shown by the indices in Table 5.2. The controlled responses, shown in Figure 5.31, are admittedly more sluggish than those based on the initial direct dual quality controllers, but the detuned bottoms composition controller was selected

Table 5.2

DUAL QUALITY CONTROLLER DESIGN

CASE	Initial Parameters		Tuned Parameters
INDIRECT	LOOP 1	K_p= -10 K_i= 0.10	
	LOOP 2	K_p= 0.012 K_i= 0.10	INITIAL PARAMETERS USED
	IAE	LOOP 1: 8.46 LOOP 2: 39.51 TOP: 0.01282 BTM: 0.03526	
DIRECT	LOOP 1	K_p= -2000 K_i= 0.10	K_p= -2000 K_i= 0.10
	LOOP 2	K_p= -4.38 K_i= 0.40	K_p= -3.00 K_i= 0.30
	IAE	TOP: 0.01929 BOT: 0.02752	TOP: 0.01919 BTM: 0.02497



QUALITY LOOP 1

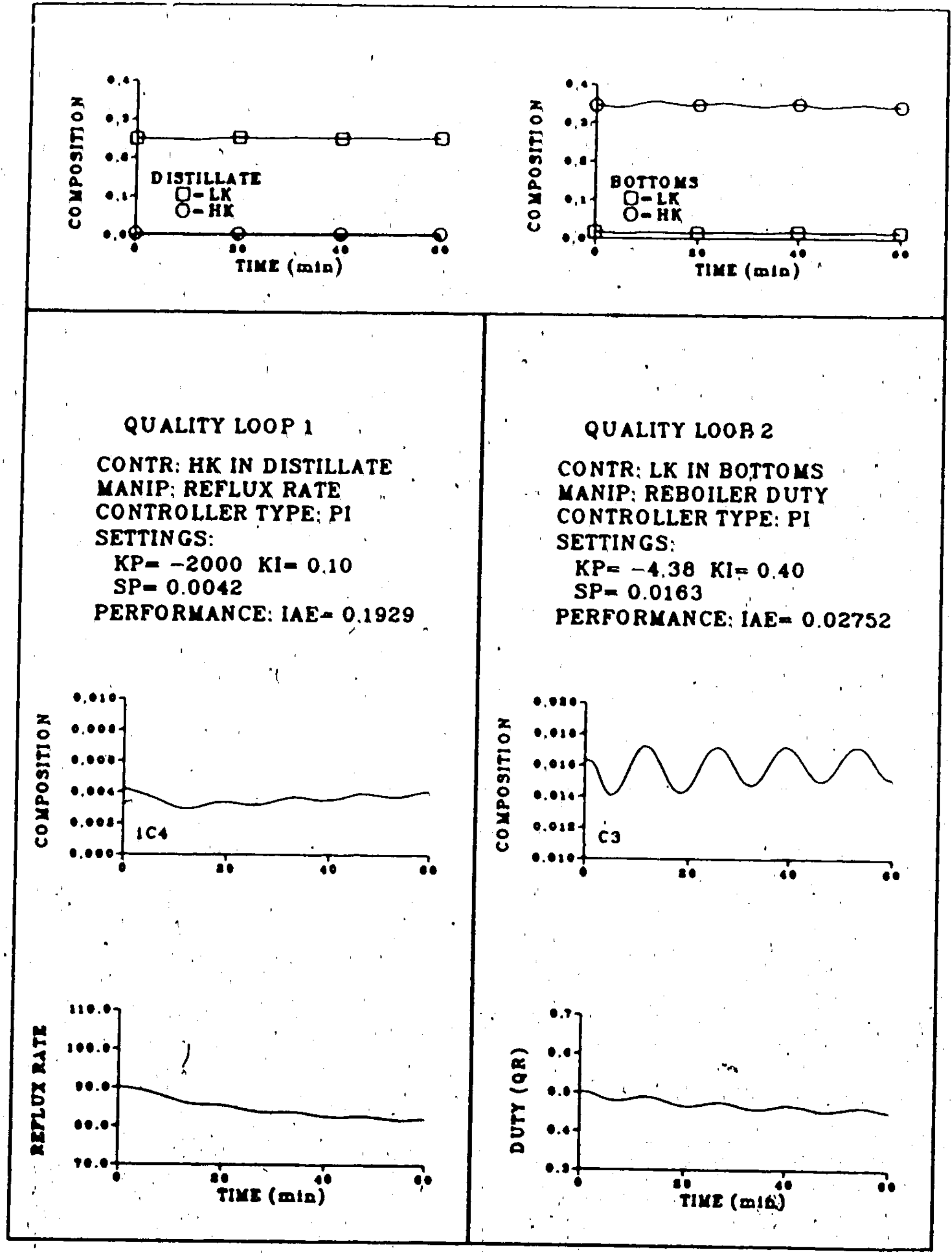
CONTR: STAGE 6 TEMP.
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -10 KI= 0.10
SP= 331.22K
PERFORMANCE: IAE= 0.01282

QUALITY LOOP 2

CONTR: STAGE 23 TEMP.
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= 0.012 KI= 0.10
SP= 368.56K
PERFORMANCE: IAE= 0.03526

Figure 5.29

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR INDIRECT DUAL QUALITY CONTROL BY COMBINING SINGLE LOOP CONTROLLERS



QUALITY LOOP 1

CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= −2000 KI= 0.10
SP= 0.0042
PERFORMANCE: IAE= 0.1929

QUALITY LOOP 2

CONTR: LK IN BOTTOMS
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= −4.38 KI= 0.40
SP= 0.0163
PERFORMANCE: IAE= 0.02752

Figure 5.30

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR DIRECT - DUAL QUALITY CONTROL BY COMBINING SINGLE LOOP CONTROLLERS for direct dual quality control on the basis of the performance indices.

It should be noted that for both direct and indirect dual quality control the trend is that better distillate composition control performance is achieved with a single loop control strategy than with a multiloop control strategy. Conversely, better bottoms composition control performance is achieved under a multiloop control scheme than under single loop control. These observations are based on the particular controllers used and no extensive tuning work was done.

The dual composition controllers were tested for effectiveness in dealing the a 10% feed rate increase disturbance. Performance indices are listed in Table 5.3 and the column responses to the disturbances are shown in Figures 5.32 and 5.33 for indirect and direct composition control respectively. The response is unstable under indirect quality control and in both cases control performance is worse than it was for the corresponding feed rate decrease case.

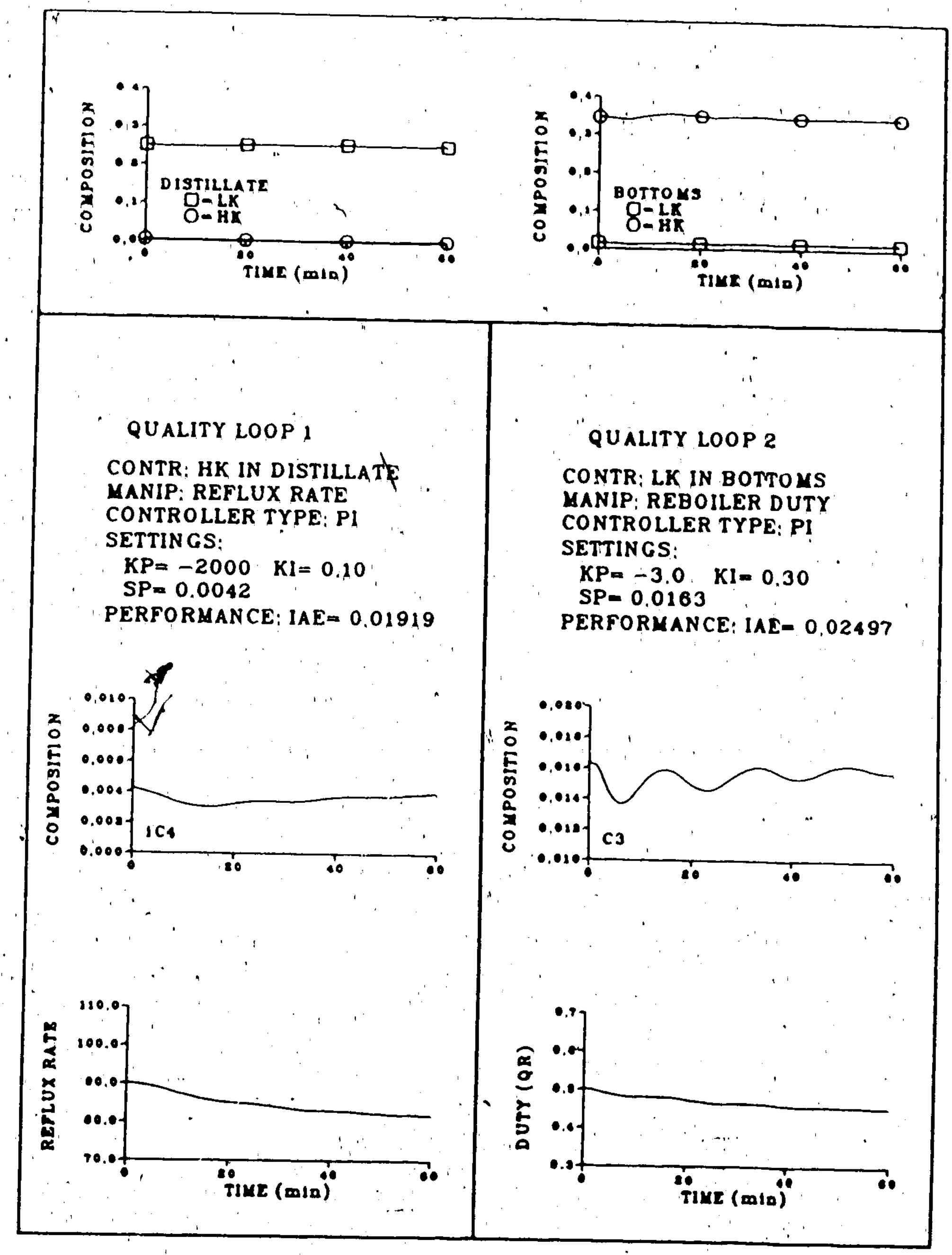
5.4.2 Interaction Analysis

Interaction between the control loops has been seen to have a different effect on control performance depending on the type of control, i. e. direct or indirect, and the type of disturbance, i. e. feed rate increase or decrease. Analysis using open loop interaction measures was performed

Table 5.3

SUMMARY OF DUAL QUALITY CONTROL PERFORMANCE FOR FEED RATE DISTURBANCES

		SINGLE LOOP			MULTILOOP	
		-10% FEED	+10% FEED		-10% FEED	+10% FEED
DIRECT						
	Loop 1 (Distillate Composition Control)					
	TOP IAE	0.00590	0.00268	TOP IAE	0.01919	0.01964
	BTM IAE	0.29647	0.75263	BTM IAE	0.02497	0.02660
	Loop 2 (Bottoms Composition Control)					
	TOP IAE	0.01492	0.06943			
	BTM IAE	0.04222	0.01792			
INDIRECT						
	Loop 1 (Distillate Composition Control)					
	TOP IAE	0.00988	0.01218	TOP IAE	0.01282	0.01454
	BTM IAE	0.26867	0.58938	BTM IAE	0.03526	0.05299
	Loop 2 (Bottoms Composition Control)					
	TOP IAE	0.03994	0.06452			
	BTM IAE	0.04230	0.03081			



QUALITY LOOP 1

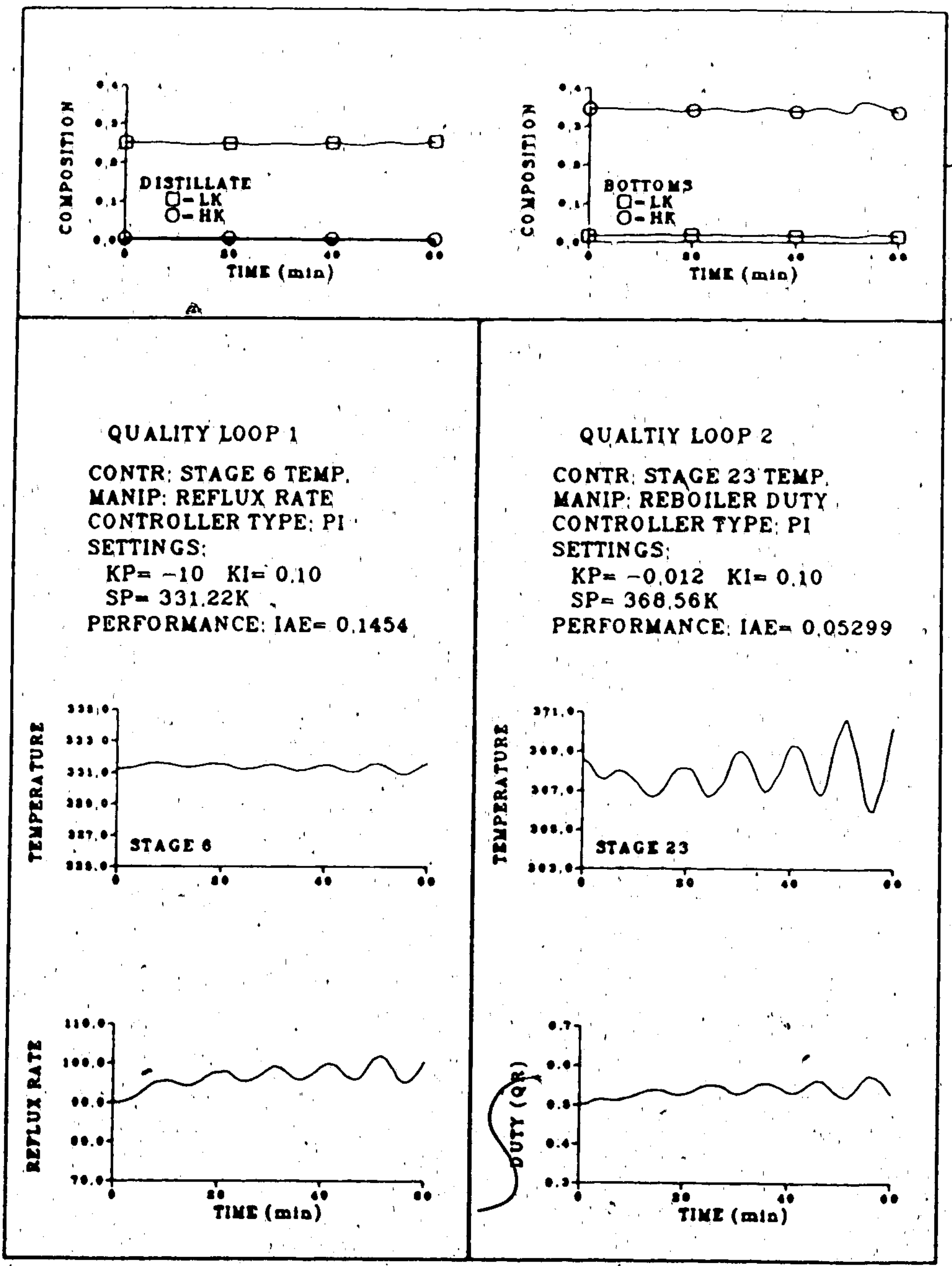
CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -2000 KI= 0.10
SP= 0.0042
PERFORMANCE: IAE= 0.01919

QUALITY LOOP 2

CONTR: LK IN BOTTOMS
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= -3.0 KI= 0.30
SP= 0.0163
PERFORMANCE: IAE= 0.02497

Figure 5.31

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR DIRECT DUAL QUALITY CONTROL AFTER DETUNING THE BOTTOMS COMPOSITION CONTROLLER



QUALITY LOOP 1

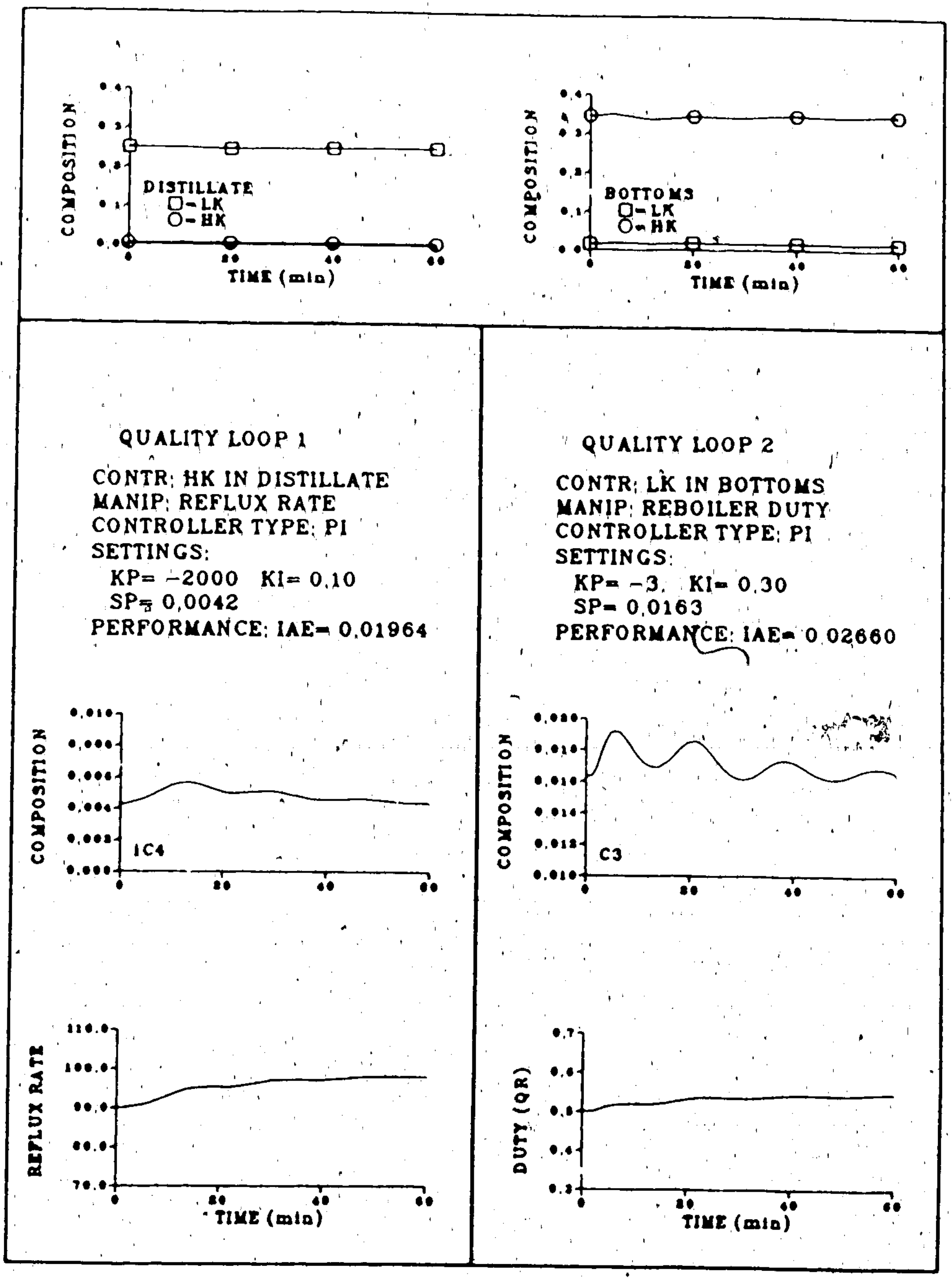
CONTR: STAGE 6 TEMP.
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= −10 KI= 0.10
SP= 331.22K
PERFORMANCE: IAE= 0.1454

QUALTIY LOOP 2

CONTR: STAGE 23 TEMP.
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= −0.012 KI= 0.10
SP= 368.56K
PERFORMANCE: IAE= 0.05299

Figure 5.32

CLOSED LOOP RESPONSES TO A 10% FEED RATE INCREASE FOR INDIRECT DUAL QUALITY CONTROL



QUALITY LOOP 1

CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: PI
SETTINGS:
KP= -2000 KI= 0.10
SP= 0,0042
PERFORMANCE: IAE= 0.01964

QUALITY LOOP 2

CONTR: LK IN BOTTOMS
MANIP: REBOILER DUTY
CONTROLLER TYPE: PI
SETTINGS:
KP= -3. KI= 0.30
SP= 0.0163
PERFORMANCE: IAE= 0.02660

Figure 5.33

CLOSED LOOP RESPONSES TO A 10% FEED RATE INCREASE FOR DIRECT DUAL QUALITY CONTROL to determine whether or not the dynamic results observed could have been predicted based on a knowledge of steady state system gains.

Relative Gain Analysis

Relative gains were calculated for direct and indirect dual composition control based on steady state gains calculated for ±.05%, ±.1%, ±1%, ±5% and ±10% perturbations in reflux rate and reboiler duty. For a 2x2 system the relative gain may be calculated as

$$\lambda = [\ 1 - \frac{K_{12}\ K_{21}}{K_{11}\ K_{22}}\ ]^{-1} \qquad (5.1)$$

where K_{ij} is the steady state gain between the i^{th} controlled variable in response to a perturbation in the j^{th} manipulated variable. A relative gain array may be constructed from the relative gains

$$\Lambda = \begin{array}{c} \\ c_1 \\ c_2 \end{array} \begin{array}{c} \begin{array}{cc} m_1 & m_2 \end{array} \\ \left[\begin{array}{cc} \lambda & 1-\lambda \\ 1-\lambda & \lambda \end{array} \right] \end{array}$$

where c_k represents the controlled variable for loop k, and m_k represents the manipulated variable for loop k. The relative gain may be used to determine appropriate pairings for controlled and manipulated variables since less interaction between loops may be expected for pairing with $\lambda \cong 1$. In addition, if $\lambda<0$ only conditional closed loop stability is expected; for $|\lambda|>>1$ the system may be extremely sensitive; and for $|\lambda|<0.5$ severe propogation between the loops can be expected due to coupling with the most severe interaction expected for $|\lambda|\cong 0$ (McAvoy, 1983; Bristol 1985).

The steady state gains for the direct and indirect dual quality control schemes considered here are listed in Table 5.4 with the relative gains calculated from them. The values of the relative gains are found to depend on both the direction and the magnitude of the manipulated variable perturbations used for the calculation.

This dependence has been previously reported in the literature. Kim and McAvoy (1982) used a steady state simulation procedure based on the Wang-Henke method to calculate relative gains. They reported that if relative gains are found to depend on the direction of perturbations then the perturbation size used was too large or the simulation convergence tolerance too loose. These workers used perturbations of magnitude .05%, .2%, .5% and 2%. Comparing results for three binary columns they found that a perturbation magnitude of 2% yielded inaccurate relative gains in the case of a high purity column (99%-1%). They recognized that a perturbation size of .05% could result in incorrect RGA values due to numerical roundoff error and recommended a perturbation size of .2% for their three example cases.

Thurston (1981) also noted a dependence of the relative gains on the direction of perturbations used to establish

Table 5.4

STEADY STATE AND RELATIVE GAINS FOR DUAL QUALITY CONTROL

Indirect Dual Quality Control

Perturbation Size (%)	K_{11}	K_{12}	K_{21}	K_{22}	λ
+ 0.05	-0.889	128	-15.7	2500	10.2
- 0.05	-0.667	164	-11.6	3140	10.6
+ 0.10	-0.811	150	-14.8	2760	148.6
- 0.10	-0.789	146	-13.3	2920	6.3
+ 1.00	-0.499	562	-9.98	2500	-0.3
- 1.00	-2.39	87.0	-12.8	1940	1.31
+ 5.00	-0.288	649	-4.30	673	-0.07
- 5.00	-3.29	50.0	-3.58	775	1.07
+ 10.0	-0.209	489	-2.54	389	-0.07
- 10.0	-2.56	37.3	-2.10	445	1.07

Direct Dual Quality Control

Perturbation Size (%)	K_{11}	K_{12}	K_{21}	K_{22}	λ
+ 0.05	-.00178	0.360	.0227	-3.60	3.63
- 0.05	-.00200	0.320	.0167	-4.60	2.39
+ 0.10	-.00178	0.380	.0219	-3.84	-4.60
- 0.10	-.00211	0.300	.0186	-4.40	2.51
+ 1.00	-.00108	1.56	.0198	-2.64	-0.10
- 1.00	-.00643	0.180	.0138	-4.03	1.11
+ 5.00	-.00055	2.76	.0157	-0.64	-0.01
- 5.00	-.01349	0.091	.0034	-2.99	1.01
+ 10.0	-.00037	2.95	.0119	-0.32	-0.003
- 10.0	-.01340	0.062	.0018	-2.17	1.00

the steady state gains. On the basis of his analysis he attributed this behaviour to "degeneracy". "Degeneracy" is said to occur when one manipulated variable has a great effect on both controlled variables, so that the second manipulated variable has little effect on the controlled variable with which it is paired (McAvoy, 1983). Using perturbations of ±1%, Thurston concluded that only single point control should be applied to the column and that this resulted in good composition control at both ends of the column. McAvoy (1983) suggested using singular value decomposition to determine whether or not decoupling is possible when degeneracy exists.

Stathaki (1982) also found that the relative gains values calculated for an industrial deethanizer column depended on the perturbation direction for perturbation magnitudes of 5% and 10%. Opposite control loop pairing was indicated for positive versus negative perturbations for steady state gains determined using column simulations. Closed loop simulation results with control loop pairing based on the negative perturbation case resulted in unstable control for a disturbance requiring that both manipulated variables increase.

Ralston (1983) calculated relative gains for an industrial column using a dynamic simulation program for manipulated variable perturbations between .05% and 2%. Since the relative gains depended on the direction of perturbation regardless of the size of perturbation, she followed the approach of Thurston (1981) in concluding that only single quality control should be used instead of dual quality control.

Referring to Table 5.4 it is seen that for perturbations made in the same direction, the relative gains based on perturbations larger than 1% are of the same order of magnitude whereas those based on perturbations smaller than 1% are inconsistent. For this reason it was assumed that sensitivity to roundoff errors made the relative gains based on perturbations of ±.05% and ±.1% inaccurate. The steady state and relative gains calculated using perturbations of ±1% of the manipulated variables were chosen as a compromise between avoiding numerical inaccuracy and obtaining reasonable estimates of the partial derivatives used in the development of the relative gain measure (McAvoy, 1983). This type of tradeoff is necessary for calculation of relative gains for any nonlinear system as was noted by Mijares *et al.* (1985). These authors did not present any recommendations for the size of perturbations to be used nor did they indicate that the relative gain calculation may have to be repeated several times for any given system to determine the appropriate perturbation size. This latter fact has a strong bearing on their shortcut calculation method which is designed to reduce the computational effort required to calculate relative gain arrays for a number of possible control structures for nonlinear systems.

Based on the control performance results shown in Figures 5.29, 5.31, 5.32 and 5.33 for feed rate disturbances, the relative gains calculated using negative perturbations of 1% or more seem more credible than those calculated using positive perturbations of the same magnitudes. Interaction is not as severe as is suggested by the small negative λ calculated using positive perturbations, even in the indirect dual quality control case in which the system is subjected to a feed rate increase (shown in Figure 5.32).

Relative Disturbance Gain

The relative disturbance gain has recently been proposed as a measure of the effect of interaction predicted using relative gain analysis (Stanley *et al.*, 1985). It involves consideration of the steady state gains in response to a disturbance in addition to those in response to perturbations in the manipulated variables. With this "disturbance gain" designated as K_{i3} for the steady state gain of the i^{th} controlled variable in response to a disturbance:

$$\beta_1 = \lambda \left(1 - \frac{K_{23}\ K_{12}}{K_{13}\ K_{22}}\right) \tag{5.2}$$

$$\beta_2 = \lambda \left(\frac{1-\beta_1}{\lambda-\beta_1}\right) \tag{5.3}$$

Table 5.5 summarizes the disturbance gains and relative disturbance gains for each loop for the direct and indirect quality control cases using perturbations of ±0.1%, ±1% and ±10% in the manipulated variables. These values were calculated using the steady state and relative gains shown in Table 5.4.

Table 5.5
DISTURBANCE GAINS AND RELATIVE DISTURBANCE GAINS FOR DUAL QUALITY CONTROL

Perturbation (%)		K_{13}	K_{23}	β_1	β_2
Direct Control	+ 0.10	0.	.0072	—	—
	− 0.10	0.	.0026	—	—
	+ 1.00	.0006	.0050	−0.06	−0.02
	− 1.00	−.0004	.0045	0.51	0.99
	+ 10.00	.0002	.0043	−0.60	−0.01
	− 10.00	−.00207	.0001	1.0	1.0
Indirect Control	+ 0.10	−.140	−4.98	−83.5	42.9
	− 0.10	0.080	−1.46	12.0	11.9
	+ 1.00	−0.028	−3.15	7.29	−0.25
	− 1.00	−0.038	−3.10	−3.48	1.23
	+ 10.00	0.036	−1.84	−4.59	−0.09
	− 10.00	−0.779	−2.85	0.74	0.84

The analysis of relative disturbance gains is based on the magnitude of the β values. If $|\beta|>1$ then larger changes in controller output are required to compensate for a disturbance in the case of dual composition control than would be required in the single loop case so the interaction detracts from control. If $|\beta|<1$ then the interacting control is advantageous in that less control action is required in the multiloop case than in the single loop case.

The magnitudes of the RDG values shown in Table 5.5 vary with the magnitude and direction of the perturbations used to calculate them due to the importance of the relative gain in Equations 5.2 and 5.3.

To evaluate the validity of the calculated relative disturbance gain values, the control action and performance indices for the dual quality control cases must be compared with those for the corresponding single quality control cases. Table 5.6 summarizes the percentage change in IAE values and the action of the manipulated variable required for dual quality control relative to single quality control. Comparison of the β values in Table 5.5 with the information in Table 5.6 shows that there is little correlation between the relative disturbance gain values and the simulated control performance. As a result, the use of these steady state operability measures provides little insight into interaction between the control loops for simultaneous control of both product streams.

5.5 Feedforward Control

Feedforward control action can be used to improve control performance as was discussed in Section 1.2. In this section results are presented for two feedback control schemes augmented with feedforward control action. As suggested in Section 1.2, feedforward action was restricted to that based on feed rate with reflux rate or reboiler duty

Table 5.6

DUAL QUALITY CONTROL ACTION AND CONTROL PERFORMANCE RELATIVE TO SINGLE QUALITY CONTROL ACTION AND CONTROL PERFORMANCE

	Feed Flow Rate Disturbance	Change in IAE Performance Index		Manipulated Variable Action: Greater (+) or Less (-) than Single Loop Case	
		Loop 1	Loop 2	Loop 1	Loop 2
INDIRECT CONTROL	- 10%	+30	-17	+	
	+ 10%	+19	+72	+	+
DIRECT CONTROL	- 10%	+227	-35	+	-
	+ 10%	+633	+48	+	+

manipulated to maintain a specified ratio to the feed rate. For these cases no dynamic feedforward compensation was used.

The two control strategies investigated are examples of single loop indirect quality control. In the first case the single loop indirect distillate composition controller discussed in Section 5.3 was used while the reboiler duty was adjusted based on the feed rate. The controlled responses to a 10% feed rate decrease are shown in Figure 5.34. Control system performance, in terms of IAE values, is compared with that achieved using only feedback control in Table 5.7. The controlled product composition control improves slightly with feedforward action and the bottom composition stays closer to the desired value.

Feedforward compensation offers even more improvement in the second case considered. This case involved the indirect feedback bottoms composition control scheme discussed in Section 5.3 with the column reflux rate adjusted to maintain a specified ratio to the feed flow rate. The responses to a 10% feed rate decrease using this scheme are shown in Figure 5.35 with IAE performance indices given in Table 5.7. Control of the bottoms composition is considerably improved and the IAE performance index for top product composition reduced by a factor of almost 10.

No optimization of the feedforward gain or retuning of the feedback controllers was performed for these cases. Use of the dynamic simulator to tune up such applications could

Table 5.7

CONTROL PERFORMANCE FOR CASES WITH AND WITHOUT FEEDFORWARD COMPENSATION

		Without Feedforward	With Feedforward
Distillate Composition Control			
	TOP IAE	.00988	.00978
	BTM IAE	.26867	.18225
Figure		5.14	5.34
Bottoms Composition Control			
	TOP IAE	.03994	.00389
	BTM IAE	.04230	.02793
Figure		5.19	5.35

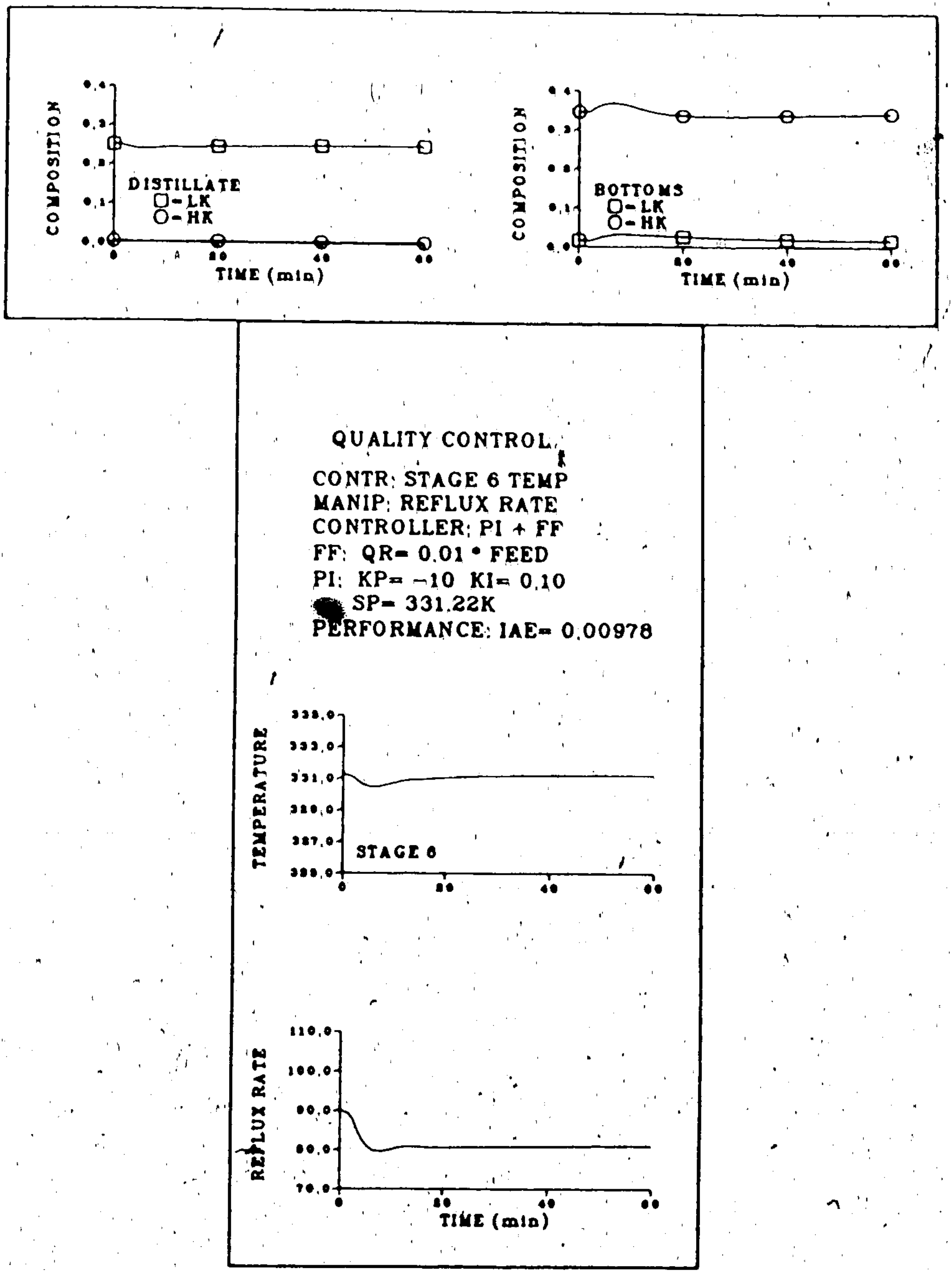
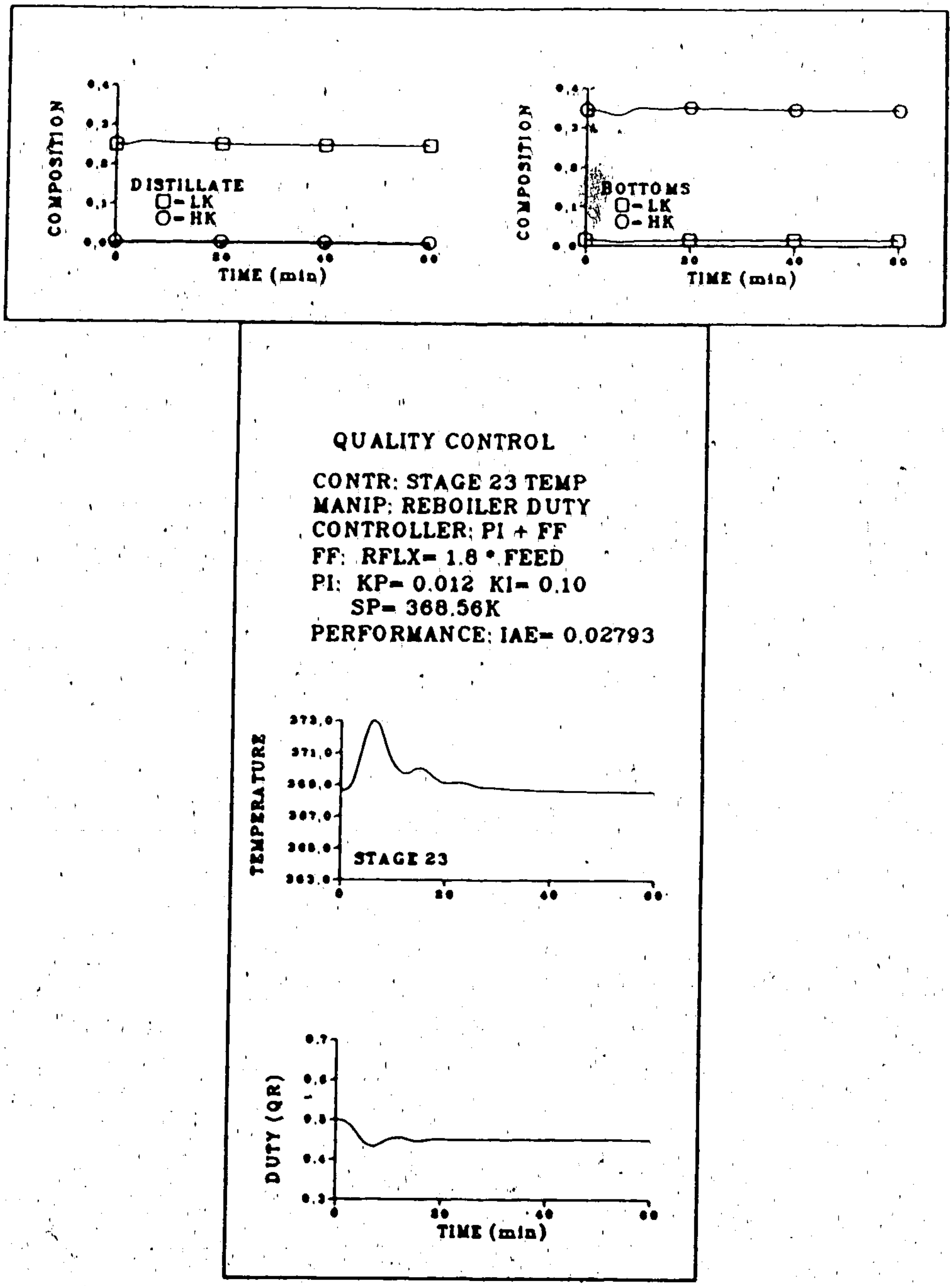


Figure 5.34

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR INDIRECT SINGLE QUALITY CONTROL OF DISTILLATE COMPOSITION WITH FEEDFORWARD COMPENSATION



QUALITY CONTROL

CONTR: STAGE 23 TEMP
MANIP: REBOILER DUTY
CONTROLLER: PI + FF
FF: RFLX= 1.8 * FEED
PI: KP= 0.012 KI= 0.10
SP= 368.56K
PERFORMANCE: IAE= 0.02793

Figure 5.35

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE FOR INDIRECT SINGLE QUALITY CONTROL OF BOTTOMS COMPOSITION WITH FEEDFORWARD COMPENSATION be helpful in an industrial situation.

5.6 Self-Tuning Control

The self-tuning control algorithm used in this study was described in Section 4.3. All cases were run for dual quality control with reflux rate manipulated to control the distillate composition and reboiler duty manipulated to control the bottoms compositions. Figure 5.36 is a schematic diagram of the control scheme used. For this work no measurement of the feed rate disturbance variable was assumed and no decoupling was implemented.

The adaptive control cases were run using inverse PI weighting on the control action, Q weighting, as was described in Section 4.3 and using the relations between PI controller parameters and inverse PI weighting parameters which are discussed in the user's manual (Carling, 1986). The parameters for the weighting polynomial were initially calculated based on the controllers designed for dual direct quality control which were discussed in Section 5.4. Some adjustments of these parameters were made in subsequent cases to improve control performance.

Model polynomial parameters were initially set to zero and were estimated during a preliminary run during which PI controllers were in effect. No attempt was made to excite the system beyond the introduction of a -10% feed rate disturbance. The parameters appeared to have converged after the one hour transient period simulated.

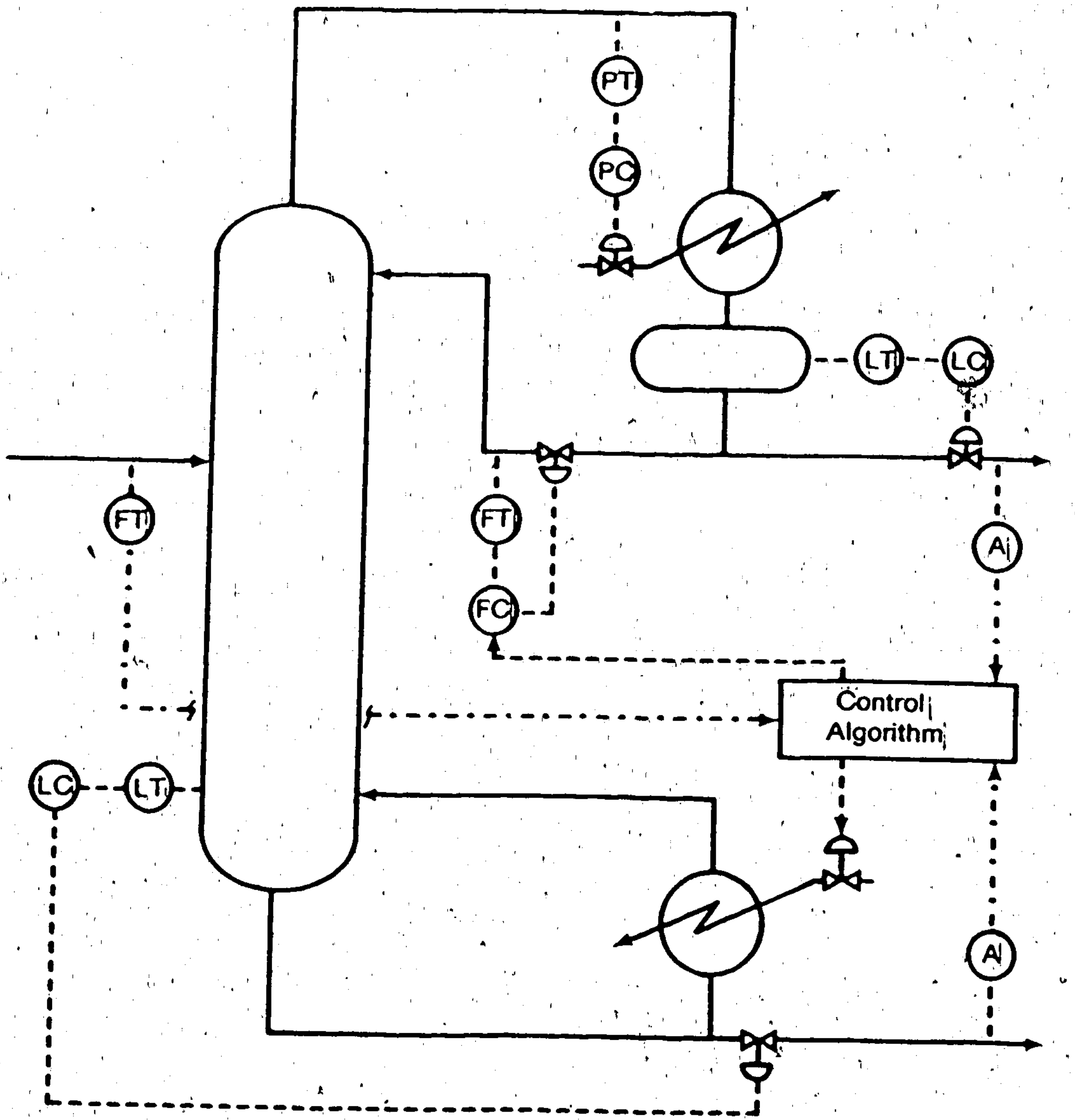


Figure 5.36

SELF TUNING CONTROL SCHEME

The model parameter estimates were then used to initialize self-tuning control for both loops. In all cases controller output limits of ±25% of the base case steady state manipulated variable values were imposed. In addition, controller output changes were limited to a set value per control interval.

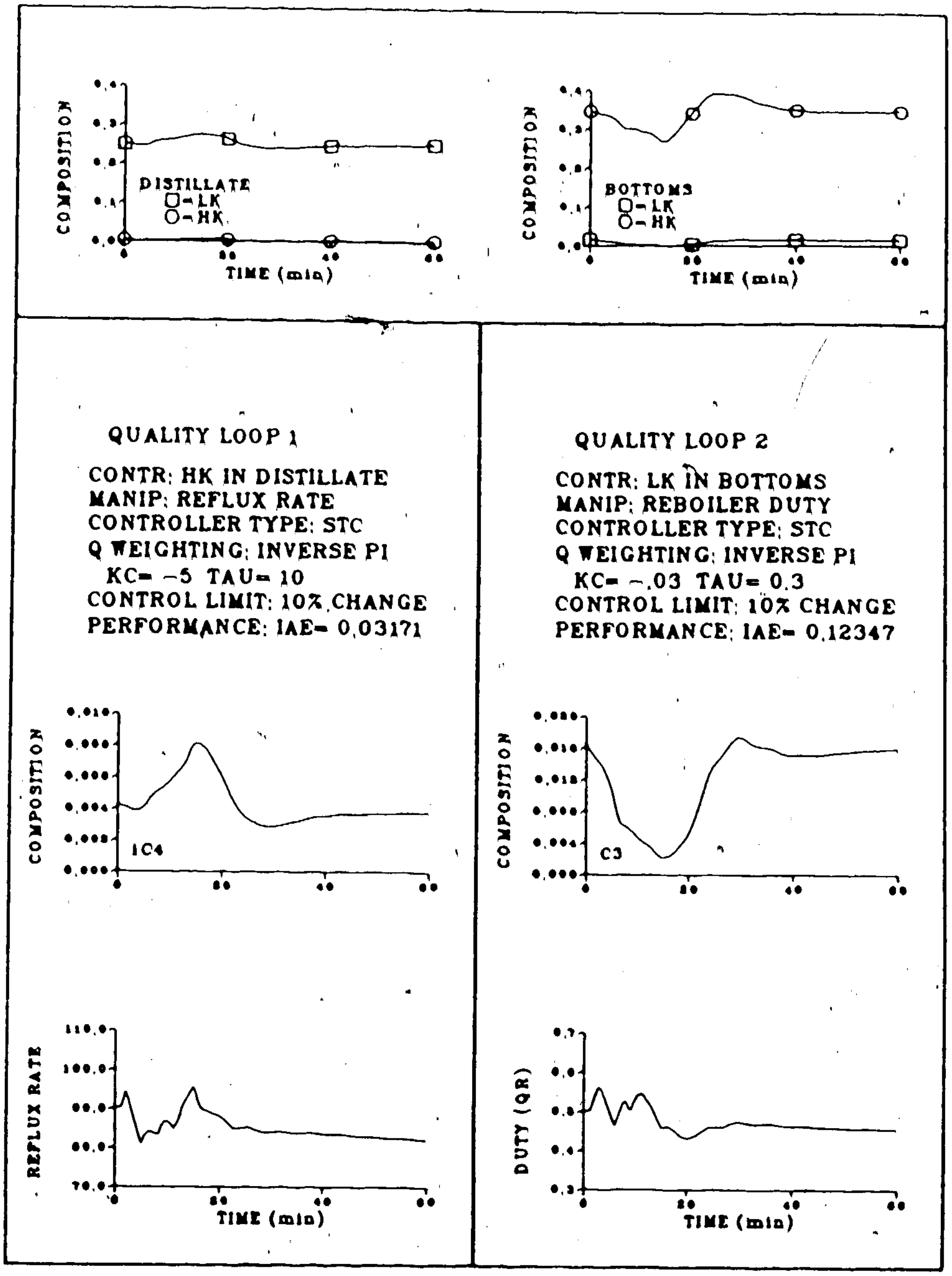
Table 5.8 summarizes the controller tuning factors and the control performance after 10% feed rate decrease disturbances for three sets of controller parameters. Figure 5.37 shows the closed loop column responses for the initial tuning factors calculated directly from the conventional direct dual quality control case. Although the overall performance is reasonable in that the controlled variables are close to their setpoints at the end of the transient, control action is extreme and erratic.

The first step taken in an attempt to improve control performance was to alter the Q weighting parameters used. The closed loop responses to a 10% feed rate disturbance after these adjustments are shown in Figure 5.38. The initial model parameters used in this case were identical to those used in the case previously discussed. As seen in Table 5.8 the performance indices calculated for this case are better than those for the initial case. The index for the top loop is lower than the corresponding index for conventional direct dual quality control while that for the bottom loop is somewhat worse. Control action is still extreme, but is more gradual than in the case with the

Table 5.8

SELF-TUNING CONTROLLER PERFORMANCE FOR -10% FEED RATE DISTURBANCES

CASE	BASIS FOR Q WEIGHTINGS	OUTPUT RANGE	OUTPUT CHANGE PER INTERVAL	PERFORMANCE
1	K = -5 TI = 10	±25%	±10%	TOP IAE: 0.03171 BTM IAE: 0.12347
2	K = -5 TI = 1	±25%	±10%	TOP IAE: 0.01723 BTM IAE: 0.14647
3	K = -5 TI = 1	±25%	±2%	TOP IAE: 0.01294 BTM IAE: 0.11067



QUALITY LOOP 1

CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: STC
Q WEIGHTING: INVERSE PI
KC= -5 TAU= 10
CONTROL LIMIT: 10% CHANGE
PERFORMANCE: IAE= 0.03171

QUALITY LOOP 2

CONTR: LK IN BOTTOMS
MANIP: REBOILER DUTY
CONTROLLER TYPE: STC
Q WEIGHTING: INVERSE PI
KC= -.03 TAU= 0.3
CONTROL LIMIT: 10% CHANGE
PERFORMANCE: IAE= 0.12347

Figure 5.37

CLOSED LOOP RESPONSES TO A 10% FEED RATE DISTURBANCE FOR SELF TUNING CONTROL WITH Q WEIGHTING BASED ON CONVENTIONAL CONTROLLER SETTINGS

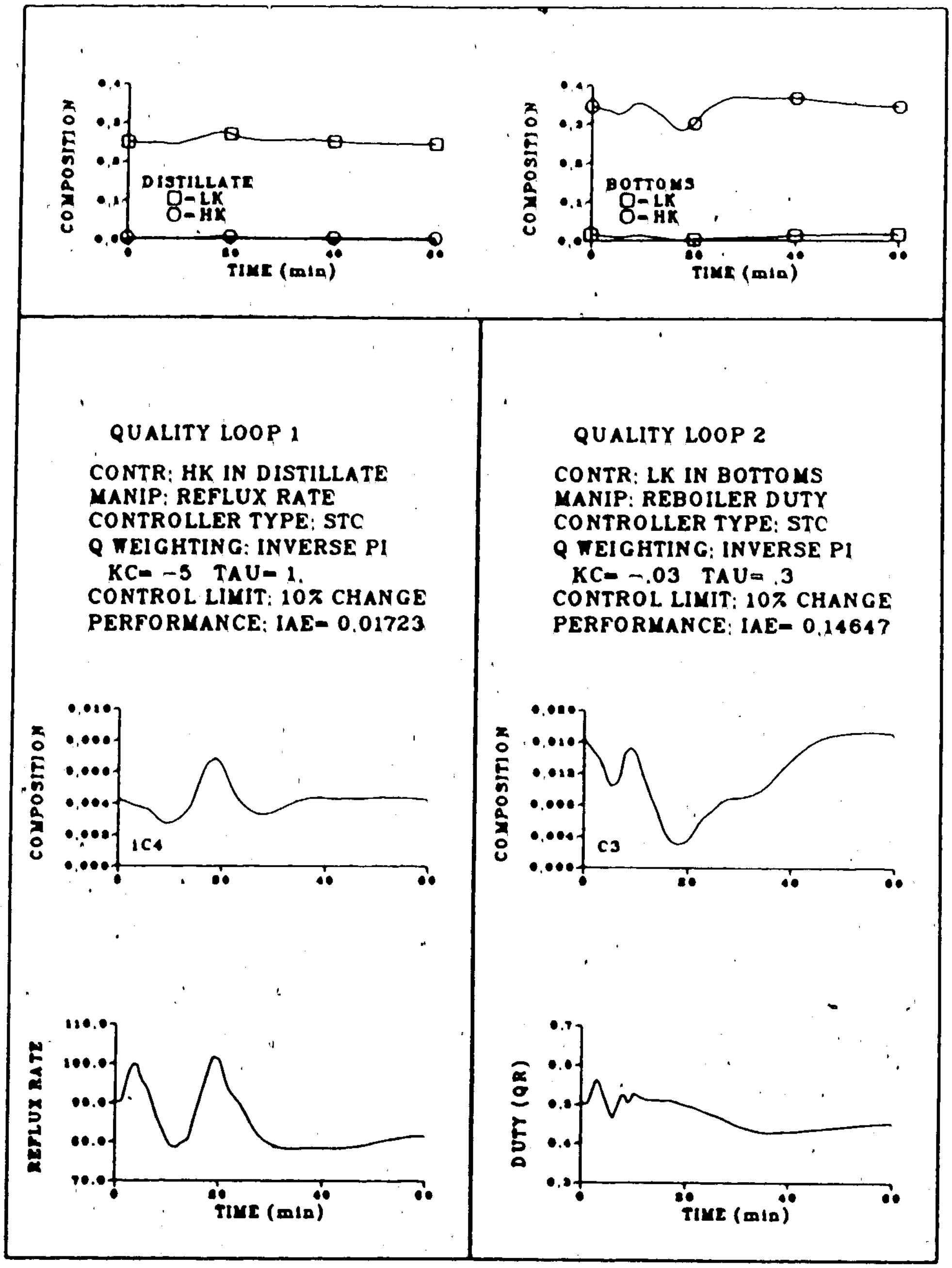
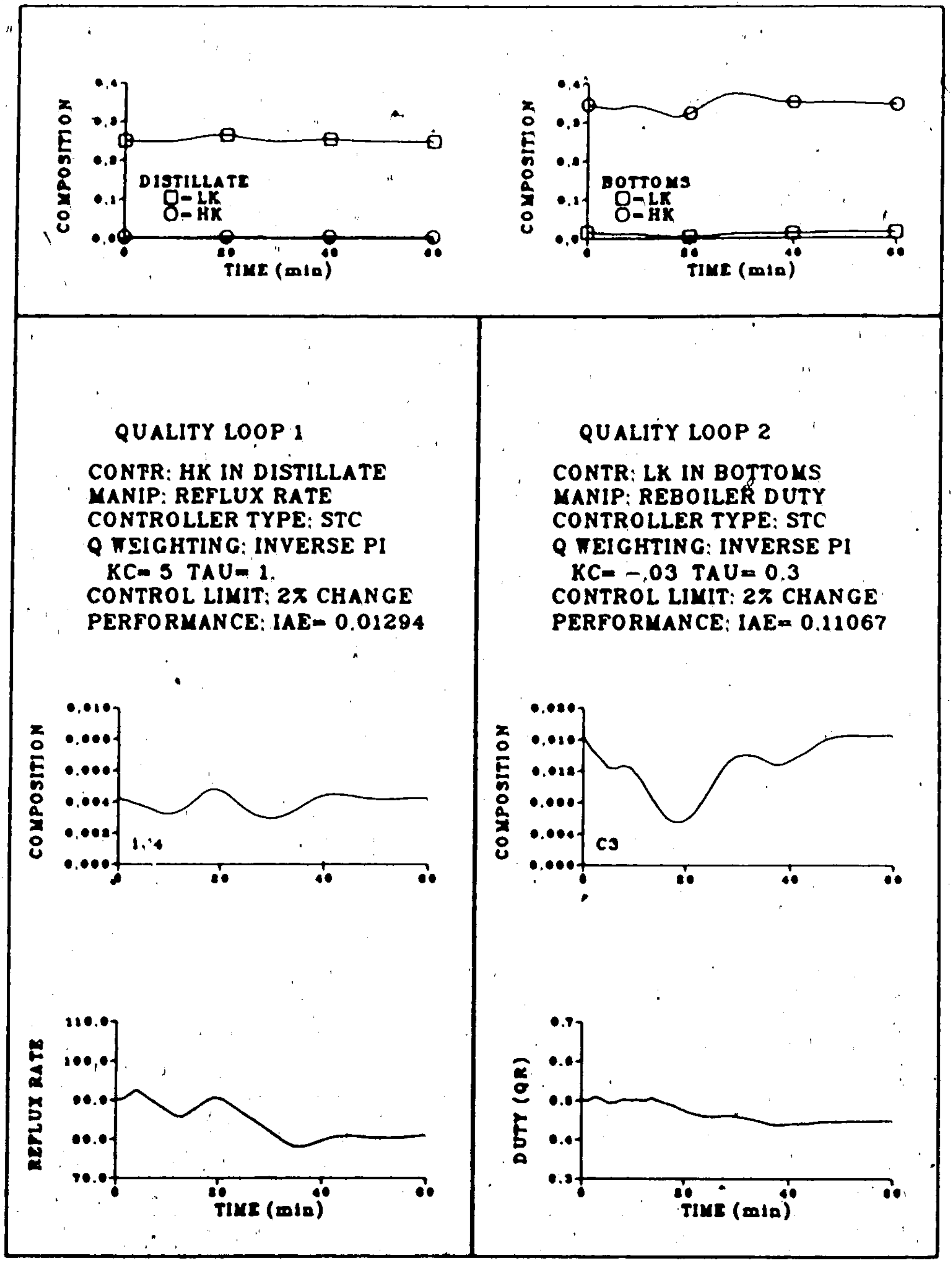


Figure 5.38

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE DISTURBANCE FOR SELF TUNING CONTROL WITH ADJUSTED Q WEIGHTING FACTORS initial Q weightings. The final self-tuning case discussed here used the same Q weightings, but restricted changes in controller output to ±2% per control interval. The closed loop responses shown in Figure 5.39 indicate that this restriction improves the control performance considerably.



QUALITY LOOP 1

CONTR: HK IN DISTILLATE
MANIP: REFLUX RATE
CONTROLLER TYPE: STC
Q WEIGHTING: INVERSE PI
KC= 5 TAU= 1.
CONTROL LIMIT: 2% CHANGE
PERFORMANCE: IAE= 0.01294

QUALITY LOOP 2

CONTR: LK IN BOTTOMS
MANIP: REBOILER DUTY
CONTROLLER TYPE: STC
Q WEIGHTING: INVERSE PI
KC= -.03 TAU= 0.3
CONTROL LIMIT: 2% CHANGE
PERFORMANCE: IAE= 0.11067

Figure 5.39

CLOSED LOOP RESPONSES TO A 10% FEED RATE DECREASE DISTURBANCE FOR SELF TUNING CONTROL WITH ADJUSTED Q WEIGHTING FACTORS AND TIGHTENED RESTRICTION ON CONTROLLER OUTPUT

6. CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

6.1 Conclusions

The DYCONDIST simulator developed at the University of Alberta has been enhanced during the course of this work. The simulator fulfils a need for a readily available, general purpose program to be used to study multicomponent distillation dynamics and control. Its development is timely in that industry is continually motivated to determine more efficient operating procedures and this requires both better understanding of the process and the ability to "experiment" with advanced control strategies without jeopardizing actual plant operations.

An effort has been made to develop a framework within which literature recommendations for distillation column control systems may be compared. This is useful since there are almost as many opinions on the control strategies to be used and the nomenclature with which to describe them as there are authors in the field.

The dynamic multicomponent distillation model in the simulator is based on a set of non-restrictive assumptions used to write heat and material balance equations. Most other aspects of the model (e. g. tray liquid holdup assumption, stage efficiency) are handled in a form which facilitates use of a number of different options.

Control algorithms have been implemented in the simulator with two basic restrictions:

1. proportional-only level controllers are assumed
2. quality controllers are implemented as remote control loops

One form of the conventional PID control algorithm has been implemented and tested as has a self-tuning control algorithm. Provision has also been made for the incorporation of user-written control algorithms.

A user's manual has been compiled to aid in the selection of program options as well as to facilitate future modifications of the simulator by fully defining program common block variables, subroutine interfaces and overall program structure. The DYCONDIST package has been enhanced by the addition of a self-standing input generator program designed to prompt the user for the input data required by the simulator. A post-processor has also been developed with which the user may select from menus of plots for data from one or more simulation cases.

Study of the open and closed loop behaviour of a depropanizer has been used to illustrate the application of the simulator to a realistic problem. Simulations performed in the course of studying column dynamic behaviour indicated inverse responses of some column compositions and temperatures. Although the phenomenon does not appear to follow any simple pattern, the following conclusions were drawn after simulation of dynamic responses to feed rate disturbances and to step changes in reflux rate and reboiler duty.

1. The number of column variables displaying inverse responses as well as the magnitude and duration of the inverse behaviour are found to depend on the disturbance variable (i. e. feed or reflux rate or reboiler duty), on the direction of the step change in the disturbance variable and on the magnitude of the step change in the disturbance variable.

2. For feed rate disturbances, feed rate decreases are more likely to result in inverse response behaviour than are feed rate increases.

3. For the most severe disturbance considered, a 30% feed rate decrease, every component displayed inverse behaviour at some location in the column. In other cases there is no instance of inverse response of the lightest component, ethane. The heaviest component, cisbutene, experiences inverse behaviour in response to feed rate decreases but not in response to feed rate increases or to step changes in reflux rate or reboiler duty.

4. Inverse responses in product stream component mole fractions in the case of feed rate disturbances are limited to the light key and lighter components in the liquid distillate and to the heavy key component in the bottoms. This agrees with the behaviour reported by Stathaki *et al.* (1985) in which inverse responses were not observed for impurity components in the product

streams.

5. Response times are seen to be asymmetric for feed rate disturbances. Response times for feed rate decreases are longer than those for feed rate increases.

6. Inverse responses are restricted to the key components for changes in reflux rate. Further, the light key inverse responses occur mainly in the rectification section whereas heavy key inverse responses occur mainly in the stripping section. The light key component shows more instances of inverse response to reflux rate decreases than to reflux rate increases, whereas the opposite is true for the heavy key component.

7. Inverse composition responses are also restricted to the key components for step changes in reboiler duty, although there are generally more instances of inverse response to reboiler duty changes than to reflux rate changes. The heavy key in the bottoms displays inverse response to decreases in reboiler duty while the light key in the distillate displays inverse response to increases in reboiler duty.

8. Inverse temperature responses are observed only for feed rate disturbances and not for changes in reflux rate or reboiler duty.

9. Inverse responses are displayed regardless of whether constant or variable stage liquid holdup is assumed.

Further study of the inverse response phenomenon involved investigation of the effect of the number and distribution of feed components on column response to a 10% feed rate decrease. A total of 11 feeds were considered with three, four or five components. As a result of this work the behaviour can be summarized as follows:

1. Inverse response behaviour is very sensitive to even small differences in feed composition.

2. Nonminimum phase behaviour is often observed in "zones" of adjacent trays and the location and size of these zones depends on the feed composition.

3. Less inverse response behaviour is observed for systems with three or four components than for systems with five feed components.

Waller and Gustaffson (1972) have stated that inverse composition responses may be observed on stages near an extremum in the composition profile for the species in question. This hypothesis was tested against the results for three, four and five component feeds and was found to represent neither a necessary nor a sufficient condition for the inverse response behaviour.

Control behaviour of the depropanizer was examined for a series of control schemes starting with a material balance or inventory control scheme and progressing to two advanced control strategies. The major objective of the study was to implement and test the control algorithms, but some additional comments may be made based on the control behaviour calculated.

Material Balance Control

Material balance control cases involved local level control at the accumulator drum and column base with the objective of ensuring gradual changes in the product flow rates so as not to upset units downstream. Reasonable performance was obtained for changes in feed rate and for changes in level setpoints. Because the level controllers are proportional-only, there was some steady state offset. Ramping setpoints would result in smoother flow changes than those resulting from step changes in setpoint and hence is desirable.

Single Quality Control

Indirect (temperature feedback) single quality control was implemented with sensors located based primarily on steady state criteria. It was found that control of distillate composition with temperature measured at stage 6 was sluggish, likely due to the lack of sensitivity of enriching section temperatures to feed rate disturbances. Control of bottoms compositions via stage 23 temperature feedback was much more responsive. Detuning of controller constants estimated using Cohen and Coon parameters improved control performance in both cases.

Direct single quality control of either stream by direct measurement of the product composition represented an improvement over indirect single quality control.

Dual Quality Control

Interaction was observed for both indirect and direct dual quality control with less deterioration experienced for the direct control case than for the indirect control case. In both cases the performance index calculated for the controlled response to a -10% feed disturbance was smaller for the bottoms composition loop than the index calculated for the corresponding single quality case. Distillate composition control was not as satisfactory under multiloop operation as for only single composition control for both feed rate increases and decreases. Performance also deteriorated in the multiloop case compared to bottoms composition control for a feed rate increase.

Interaction analysis using steady state operability measures was attempted to determine the usefulness of these measures for analyzing the control behaviour of the depropanizer. It was found that neither relative gains nor relative disturbance gains were very helpful since the relative gains calculated depended on the direction of the perturbations used to calculate the steady state gains. The conclusion which some other workers (e. g. Thurston, 1981; Ralston, 1983) had drawn from this "degeneracy" result is that dual quality control should not be attempted where the relative gains depend on perturbation direction. In this case direct dual quality control provided reasonable response to feed rate increase and decrease disturbances, and indirect dual quality control provided oscillatory control for a feed rate decrease and unstable control for a feed rate increase. Although the fact that these results were obtained without an attempt to optimally tune the controllers may have an effect on the closed loop simulations, there is little correlation between the simulation and interaction analysis results for this case.

Feedforward Control

Control performance was evaluated for two simple feedforward schemes and was found to improve performance significantly over the cases without feedforward action.

Self-Tuning Control

Cases were run to implement and test the self-tuning controller but, as for the other control cases, little time was spent on optimizing controller parameters. Control performance for the best self-tuning control case was comparable to the conventional dual quality control cases. It seems likely that this could be further improved after experimenting with control limits and weightings as literature reports consistently cite sensitivity of self-tuning control performance to algorithm parameters.

6.2 Recommendations for Future Work

It has not been possible during the course of this work to investigate all of the avenues of potentially instructive study which have been encountered. The recommendations for future work contained in this section have been divided into three sections: the first deals with possible modifications to the simulator, the second with further distillation dynamics studies, and the third with further studies of control behaviour.

6.2.1 DYCONDIST Modifications

As has been emphasized throughout this thesis, the simulator is designed to be a general purpose package for dynamic multicomponent distillation column simulation. This objective should be kept in mind as modifications are considered. It is suggested that if a change cannot be handled conveniently by replacing or modifying fewer than about ten program modules, or if it is a change that requires that the basic solution procedure be modified, then development of a parallel program rather than revision of the existing program should be considered. For example, replacement of the integration routine would require replacement of a large portion of code, but would not violate the solution procedure and so could be handled quite conveniently within the framework of the existing simulator. Study of azeotropic or extractive distillation, on the other hand, would require changes to the routines involved in the equilibrium equations as well as changes to the data structures to account for two liquid phases. Such a change might be better handled in a parallel program in which many of the peripheral subroutines from DYCONDIST could be used.

A further suggestion for those who may modify the programs in the future is that the user's manual will be useful only if updated to reflect changes in available options and required simulator input. Further, the program structure diagram and tables of common block and interface definitions contained in the manual should be updated regularly to reflect the current stucture of the simulator.

(a) Modification of ASIRK integration algorithm:

Prokopakis and Seider (1981) stated that the estimate of the derivative $\frac{\partial y_j}{\partial y_s}$ used in the estimation of the pseudo-eigenvalue of the stiffest equation should be of higher order than the simple first order estimate used in DYCONDIST. To date no apparent problems have been caused by using the lower order estimate, but a more conservative approach would be to use a higher order estimate. Since the use of the estimate procedure suggested by Prokopakis and Seider involves more computation, the alternative could be made available as an option for comparison with results calculated using the simpler approach.

(b) Dynamics of control elements:

The dynamics of control elements have not been included in the present simulator. Addition of this feature would require integration to solve the differential equations written to model the true dynamics of each loop. While adding considerably to the complexity of the model and detracting from the generality of the simulator, it may be necessary to incorporate at least an approximation of control loop dynamics in order to match plant data.

(c) Reboiler dynamics:

Since many different reboiler types exist, it may be necessary to model reboiler dynamics more accurately for some applications than is possible with the options now incorporated in the simulator. The options which are currently available are:

1. constant heat input
2. heat input calculated as a function of an overall heat transfer coefficient with optional correction of the heat transfer coefficient based on the bottoms temperature

Adding a model to account for a specific reboiler configuration would be possible, but a smaller integration time step could be forced for the entire column if the reboiler dynamics resulted in greater rates of change of the column base variables than of the overall column hydraulics.

(d) Application of loads during transient period:

The current version of the simulation is designed so that up to five disturbances may be applied at time t=0. For cases of pure dynamics this offers sufficient flexibility since any case can be stopped at time $t=t_1$ then restarted with application of a load at time t=0 of the continued run to simulate the effect of a single transient with disturbance at time $t=t_1$. For column control studies this approach is not possible unless the program is modified so that the restart data file contains the values of controller error integrals. Greater flexibility would be provided by making it possible to apply disturbances at times other than t=0. Load application times could be restricted to multiples of the sampling interval to avoid undue complexity.

(e) Setpoint ramping:

A small modification similar to that described in part (d) would provide the capability of ramping setpoints. A limited number of setpoint changes could be specified, but this number would have to be sufficiently large to ensure that ramps could be made over a reasonable length of time.

(f) Independent integration of local control loops:

The integration of local controller differential equations is currently tied to the integration of the column liquid hydraulic equations. In order to allow a smaller time step for controller ODE integration, an additional integration would have to be performed to solve for the dynamics of the local control variables from the beginning to the end of the time step used for the liquid rates calculation.

(g) Efficiency correlations:

It is appropriate for many columns to assume a different efficiency for each column section. For these cases it would be useful to be able to specify efficiencies on a stage-by-stage basis as is possible for the stage heat loss correlation.

6.2.2 Distillation Dynamics

(a) Verification of open loop data:

The single most important recommendation for future work is that every attempt be made to obtain dynamic test data for an operating multicomponent column in order to verify the open loop dynamic behaviour predicted by the simulator. Experimental verification has been performed (Wong, 1985) for a binary column, but it is the inverse response behaviour predicted for multicomponent mixtures which is of the greatest interest.

(b) Alternative thermodynamic behaviour representation for the depropanizer:

Although the polynomial correlations used for component enthalpies and equilibrium ratios check well against NGPA handbook data, simulation results based on these correlations could be compared with results based on a nonideal component behaviour model. This change should have little effect since large interaction effects are not expected for the components in the system.

(c) Depropanizer feed point location:

Since the depropanizer rectification section temperatures show only a very small variation from stage to stage it would be more efficient to remove some stages, effectively moving the feed point up the tower. This might have an effect on the column dynamic behaviour as more separation would occur on each stage.

(d) Development of reduced models:

By simulating column pulse tests, DYCONDIST could be used to develop reduced distillation models such as would be suitable for some advanced control applications.

(e) Automatic identification of inverse responses:

Given the limitations (cited in Chapter 3) of the routine used to identify inverse responses in this work, it is desirable that alternative identification procedures be considered. For example, to avoid missing an inverse response that begins after an initial lag, the routine could be designed with the following logic. If the initial transient value of a variable is the same as the initial value (or effectively the same), then the second transient value should be checked, and so on. The problem with this logic is that some variables might not vary significantly from the initial value throughout the transient. A "reasonable" lag could be specified to avoid excessive computation. This procedure could still be expensive and it may be worthwhile to restrict the number of variables to be checked.

(f) Depropanizer inverse response:

Changes in feed and reflux rate and reboiler duty have been seen to cause some inverse temperature and component mole fraction responses depending on the type, magnitude and direction of the disturbance, as well as the number and distribution of feed stream components. Simulation of column responses to other disturbances, such as changes in feed temperature and/or composition, would provide a more complete understanding of dynamic column behaviour and the conditions under which inverse response might be expected.

(g) Depropanizer asymmetric response times:

Wong (1985) concluded that the depropanizer dynamic response times displayed little asymmetry and little attention has been paid to response time in the course of this work. The ±30% feed disturbance cases did have product composition response times dependent on the direction of the load. This phenomenon could be considered in relation a study (Stathaki *et al.*, 1985) in which slower dynamics were observed for transients toward a steady state representing greater separation of the key components than for cases in which a disturbance forced operation away from a steady state with greater separation.

(h) Mechanism for inverse response:

The inverse temperature and composition responses must be caused by at least two opposing driving forces with one action initially dominating until it is overcome by the second force. Simplifying the dynamic distillation problem by considering a system with as few components and as few stages as possible may be helpful in identifying the driving forces responsible. A ternary feed mixture could be used in such a study since inverse responses have not been observed in binary systems, but have been seen to exist for some three component systems depending on the disturbance to which the system is subjected.

6.2.3 Distillation Control

(a) Self-tuning control study:

Since the contribution of the simulator to the field of process control is likely to be in experimentation with advanced control techniques, future work could involve further study of the self-tuning control algorithm used in the depropanizer control study. In particular, it is likely that control performance could be greatly improved by optimization of the Q, R and P weighting polynomials.

(b) Interaction analysis:

Frequency domain interaction analysis methods may provide a better indication of interaction than did the steady state methods examined in this work. If frequency domain techniques such as the inverse Nyquist array methods were to be studied, then simple transfer function models would be required (see part (d) of Section 6.2.2).

(c) Feedforward control schemes:

The feedforward control results presented in this work did not represent an extensive study of possible feedforward schemes. Comparison with other feedforward strategies would be useful. Algorithms combining feedforward and feedback action on a single manipulated variable have not yet been considered, nor has any form of dynamic feedforward compensation.

(d) Measurement delays and noise:

Provision has been made for these options, but their effect has not been considered in the control results presented here. Measurement delays affect the results showing the superiority of direct over indirect control schemes. They would likely also have a greater effect on conventional schemes than on the advanced strategies based on delayed analysis information.

(e) Temperature sensor location and inverse response:

The temperature sensor locations used in this work did not coincide with stages predicted as displaying inverse temperature response to feed disturbances. The effect of inverse response of a controlled variable on control performance could be studied by examining use of a tray with inverse temperature response as the control point for temperature feedback control.

(f) Pressure control:

Examination of column pressure control strategies could be worthwhile, especially as a means of determining what incentives exist for changing column operating conditions. For the depropanizer case this would require component equilibrium ratio correlations which are functions of both temperature and pressure instead of the current correlations which are functions of temperature only.

(g) Level control options:

The level control options implemented in the present version of DYCONDIST are limited since each option requires different modifications of the Jacobian used in the integration of the column material balance equations. The number of options should gradually be expanded to provide greater flexibility in designing an overall control system.

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Appendix A: THERMODYNAMIC DATA FOR DEPROPANIZER

Liquid Enthalpy Correlations

$h_i = a_{0i} + a_{1i}T$ (h_i in kJ/kmol, T in K)

Component	a_0	a_1
Ethane	-3.0507	0.0401130
Propylene	-3.5076	0.0459864
Propane	-5.4807	0.0538260
Isobutane	-7.7433	0.0685440
Cisbutene	-3.8991	0.0595890

Vapour Enthalpy Correlations

$H_i = b_{0i} + b_{1i}T + b_{2i}T^2$ (H_i in kJ/kmol, T in K)

Component	b_0	b_1	b_2
Ethane	6.8462	0.0199386	-0.42279
Propylene	9.6623	0.0185670	0.62658
Propane	10.542	0.0138070	2.0643
Isobutane	13.426	0.0094772	4.3614
Cisbutene	17.347	0.0022633	4.4485

Equilibrium Ratio Correlations

$$\ln(K_i) = c_{0i} + \frac{c_{1i}}{T} + \frac{c_{2i}}{T^2} \quad (T \text{ in K})$$

Component	c_0	c_1	c_2
Ethane	-3.9690	4.21544	-0.88222
Propylene	-0.70564	1.86111	-0.53390
Propane	-0.76958	1.92822	-0.56053
Isobutane	2.2268	-0.167722	-0.25249
Cisbutene	1.9634	-0.174340	-0.31756