Control Of A Binary Distillation Column Using Nonlinear Composition Estimators.

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CONTROL OF A BINARY DISTILLATION COLUMN USING NONLINEAR COMPOSITION ESTIMATORS

by

Mahendra Shah

A Dissertation
Presented to the Graduate Committee
of Lehigh University
in Candidacy for the Degree of
Doctor of Philosophy
in
Chemical Engineering

Lehigh University
1978

CERTIFICATE OF APPROVAL

Approved and recommended for acceptance as a dissertation in partial fulfillment for the requirement for the degree of Doctor of Philosophy.

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1. ABSTRACT

Indirect composition control of industrial distillation columns is frequently practiced because of difficulties associated with direct composition measurements.

Static nonlinear rigorous estimators which involve tray to tray energy and material balances were developed for product composition estimation. Another type of approximate nonlinear estimator based on statistical analysis of binary column steady state data was proposed. Criteria to select optimum secondary measurements were developed for these estimators. By steady state simulation of a constant relative volatility binary distillation column, the sensitivity of rigorous estimators to measurement errors was studied.

A steady state computer program for a pilot scale, 24 tray, methanol/water distillation column was developed. This was used to design various estimators and to evaluate steady state composition errors associated with nonlinear estimators, Brosilow's linear estimator and conventional constant tray temperature control for changes in feed composition and product composition setpoints. The steady state composition errors were negligibly small for estimator based control schemes in face of feed composition changes. It was found that for bottom's composition set point changes, steady state composition error was significant for Brosilow's linear estimator.

A dynamic program for the distillation column was also developed. The dynamic response of the column in face of feed composition and/or product composition set point changes was studied for comparative evaluation of control schemes using composition estimators and conventional composition control techniques.

The control schemes using Brosilow's linear estimator and nonlinear rigorous estimator were experimentally implemented using PDP 11/40 computer. The superiority of the control scheme using the rigorous nonlinear estimator was verified experimentally.

2. INTRODUCTION

In general, the purpose of distillation column control is to maintain the desired product quality. Conventional design of a feedback control system requires continuous measurement of product composition. However, direct measurement of product quality is difficult, expensive and, at times, unreliable. Sometimes, adequate technology to measure the product quality simply does not exist. Frequently, large measurement lags associated with composition measurement do not permit the design of an effective feedback control system. One solution to this problem is to infer product quality using convenient secondary measurements.

In distillation columns, tray temperatures and process flow rates are convenient secondary measurements. They are easily measurable and measurement errors and measurement lags are small.

2.1 Background

A large number of industrial columns are monitored using tray temperatures for indirect composition control. Extensive literature is available on temperature control of distillation columns.

A common control technique is to control the temperature of an optimum tray near the end of the column where the product is withdrawn. An optimum tray is selected such that the steady state deviation of controlled product composition is as small as possible with the restriction that the tray temperature changes due to load disturbances are greater than the sensitivity of the temperature sensor element. When the pressure variations are large enough to significantly affect the control tray temperature, pressure compensated tray temperature is used.

Another popular control scheme to offset the undesirable effects of absolute pressure variations in the column is to control a tray temperature differential, i.e. difference between two tray temperatures in some section of the column (1,2). Luyben (3) has shown that for a 25-tray deisobutanizer, the steady state error due to feed disturbances and column pressure variations is less with double differential temperature control than with conventional control techniques mentioned earlier. The double differential temperature control means to control the difference between two temperature differences in the section of the column where the product is withdrawn. Boyd (4) has demonstrated that for a fractionation column, controlling the difference between two differential temperature measurements in each section of the column reduces the steady state composition error due to process disturbances and the control system stability is increased compared with convention control systems mentioned earlier. Luyben (5) has recommended profile position control for distillation columns with sharp temperature profiles. The profile position is obtained by measuring a number of tray temperatures. Weber et al. (12,13) have proposed more sophisticated distillation column control techniques which use plural tray temperatures to maintain product compositions. One technique uses the sum of two or more selected tray temperatures to adjust key control variables. Another technique uses the sum of two selected tray temperatures to adjust one operating variable and the sum of difference of two tray temperatures and a correction factor proportional to the ratio of overhead product rate and feed rate to manipulate the second operating variable. These techniques are recommended for one feed, two product distillation columns and are superior to conventional single tray temperature measurements and material balance controls.

With recent advances in computer control technology and lower cost of control computers, studies of the application of modern control theory to multivariable chemical processes have begun. King (6) and Nu, et al., (7) have successfully applied modern concepts of control design for indirect composition control on pilot scale distillation columns. The improvement was attributed to recognition of interaction between process variables by modern control theory. However, application of such a rigorous approach to control industrial columns would be too complex and impractical considering the large number of measurements and large amount of computations needed.

Brosilow (8,15) proposed a linear static estimator using a linear combination of selected tray temperatures and steam and reflux flow rates to estimate the product quality. He demonstrated by digital simulation that application of such an estimator based control scheme to multicomponent distillation column achieved composition control comparable to that achieved with instantaneous composition measurements. Babu, et al., (9) reported that inferential composition control of an industrial debutanizer column using Brosilow's estimator gave better control than with the conventional technique of controlling a tray temperature.

2.2 Scope of Work

For a distillation column at steady state, the column is completely specified if the number of process variables measured is equal to the degrees of freedom of the column. The process variables could include feed composition, product composition, tray temperatures and process flow rates. Product composition can be estimated using a rigorous steady state mathematical model if sufficient number of tray temperatures and/or process flow rates are known (equal to or greater than the degrees of freedom of the system)

A static mathematical model for the distillation column involving tray to tray energy and material balances could be used in conjunction with selected, easily measurable process variables to estimate product quality. Composition estimation errors would be caused by

1) Modelling Errors: Composition estimation error due to inaccuracy of mathematical model describing the distillation column. One solution is to use a rigorous mathematical model for the column and periodically update column parameters.

2) Measurement Errors: Composition estimation error due to noise present in process measurements and due to sensitivity limitation of the measuring device. These could be reduced by filtering noisy measurements and proper selection of secondary measurements.

3) Dynamics of the Column: Composition estimators are based on the asumption that the column is at steady state. However, this is not true when the column is under transient condition. This error could be reduced by judicious choice of process measurements to be used in the estimator.

The present research is aimed at design of static nonlinear composition estimators which use selected tray temperatures and/or process flow rate measurements. The mathematical model is of a fundamental type involving tray to tray energy and material balances and vapor-liquid equilibrium relationships. Such an estimator would be able to handle process nonlinearities better than Brosilow's linear estimator.

The following was the proposed plan of work:

1) Develop a criterion for selecting a subset of available tray temperatures and process flow rates which when used in conjunction with a static, rigorous mathematical model would give an estimate of product quality for a binary distillation column.

2) Investigate the application of this composition control strategy to a binary distillation column by digital simulation. Compare it with Brosilow's linear estimator and conventional composition control techniques for a binary distillation column by digital simulation.

3) Conduct an experimental study on the application of this control scheme to a 24 tray, methanol/water distillation column. PDP 11/40 computer was used for real-time control.

4) Explore the extension of this control scheme using nonlinear estimators to multicomponent distillation columns.

3. BROSILOW'S LINEAR ESTIMATOR

3.1. Theory (8,15)

As mentioned earlier, the control of many chemical processes is complicated because direct product composition measurement is difficult and the process is subject to unmeasurable process disturbances. Weber and Brosilow (8) suggested that one solution to this problem is to estimate the product compositions using secondary measurements. A static estimator which estimates the product composition from a linear combination of selective process input and output measurements was developed. The static estimator is based on the static linear input-output relationship model for the process. A criterion for selecting a subset of available (easily measurable) input and output variables so as to minimize composition estimation error due to measurement errors and modelling errors was also developed.

The static estimator relates perturbations in measured quantities to perturbations in the product quality. The linear model of the process (valid in the region about a steady state operating point) is represented by

$$x = Fv = Mm + Ju \quad \dim(v) = \dim(u) + \dim(m) \qquad (1)$$

$$y = Hx = Qm + Ru \quad \dim(y) \geq \dim(u) \qquad (2)$$

$$w = Gx = Pm + Ku \qquad (3)$$

where

v = process input perturbation

u = unmeasured component of v

w = process product quality perturbation

x = process state perturbation

y = measurable process output perturbation.

Capital letters in Eq. (1), Eq. (2) and Eq. (3) are matrices and

$$(M:J) = F; \; Q = HM; \; R = HJ; \; P = GM; \; K = GJ$$

Another restriction on this linear model is that the rank of matrix R is equal to dim(u).

Using Eq. (1), Eq. (2) and Eq. (3), we get

$$w = Pm + K\hat{R}^{-1}(\hat{y}-\hat{Q}m)$$

where

$\hat{y} \equiv$ the vector of measurements selected for use in the estimator.

$\hat{R} \equiv$ the reduced model matrix (the submatrix of R formed by selecting rows of R corresponding to the measurements of $\hat{y}$).

$\hat{Q} \equiv$ the submatrix of Q associated with measurements $\hat{y}$.

However, the estimator designed might give poor estimates due to errors in modelling and measurements.

Eq. (2) could be modified to incorporate modelling errors and measurement errors.

$$(\hat{R} + \hat{E})u = \hat{b} + \hat{\varepsilon} \qquad (5)$$

where

$\hat{R} \equiv$ the error free reduced matrix

$\hat{E} \equiv$ error matrix associated with R

$\hat{b} =$ the noise free measurement vector

$\hat{\varepsilon} =$ vector sum of measurement noise in $\hat{y}$ and $\hat{Q}_m$.

u = noise estimate of the true process inputs

From Eq. (5)

$$u = \hat{R}^{+}\hat{\hat{b}} \qquad (6)$$

where

$$\hat{R}^{+} = (P\hat{\hat{R}})^{-1}P \qquad (7)$$

where $\hat{\hat{R}} = \hat{R} + \hat{E}$

$\hat{R}^{+} \equiv$ a generalized inverse of R

$P \equiv$ any matrix such that

$P\hat{R}$ is nonsingular

$\hat{\hat{b}} = \hat{b} + \hat{E}$

It can be shown that

$$\frac{||u-U||}{||u||} = \text{Cond}(\hat{R}) \frac{||\hat{E}u+\hat{\varepsilon}||}{||\dot{\hat{b}}||}$$

$\dot{\hat{b}}$ = projection of $\hat{b}$ on the space spanned by the columns of $\hat{R}$.

Large condition numbers imply high sensitivity to modelling errors. Condition numbers higher than 100 imply large errors in estimates of u due to modelling errors. If the condition number is less than 10, error amplification due to modelling error would not be significant.

To select between measurement sets, the measurement set with the lowest condition number is selected if the condition numbers vary widely. If the condition numbers do not vary widely, then the error statistics of measurements is also considered in choosing an optimum measurement set.

However, since there is a significant computation involved in calculation of condition numbers, an alternative criterion involving minimax row dot product, which selects the set of measurements with large angles between each other, is recommended by Weber and Brosilow. The cosine of angle between the two vectors is given by the normal dot product which is defined as

$$DP(i,j) = \frac{<\gamma_i,\gamma_j>}{<\gamma_i,\gamma_i>^{\frac{1}{2}}<\gamma_i,\gamma_j>^{\frac{1}{2}}} \quad i,j = 1,n$$

where

$<\gamma_i\gamma_j>$ = inner product of γ_i with γ_j

γ_i = i^{th} row of R

n = the number of feasible measurements

In order to compare various sets of measurements, we define

$$MDP_k = \max_{i,j \varepsilon S_k} DP(i,j)$$

$\equiv$ maximum row dot product of k^{th} set of measurements.

The sets of measurements with the smallest maximum row dot products are candidates for use in the estimator. The set with the lowest condition number is selected. If two or more of these sets have low condition numbers, then the set with the lowest measurement noise level is selected. If the condition numbers for all sets are very high, then the measurements in the set S_k is increased by one. The procedure is repeated until a set of measurements with an acceptable conditon number is found.

By digital simulation of a multicomponent distillation column, Brosilow showed that the composition control achieved by using Brosilow's linear estimator was comparable to that achieved with instantaneous composition measurements and superior to that achieved by controlling a tray temperature.

Brosilow's composition estimation technique is based on the assumption that the process can be adequately represented by a linear model. Generally, this is reasonable if the process is not subject to large variations in load disturbances, composition set points or system parameters. However, for a nonlinear process subject to large environmental changes, such an estimator would give large steady state composition errors.

Also, the criterion for selecting the optimum subset of the available measurements does not take into account the dynamics of the process.

3.2. Design of Brosilow's Composition Estimator

The procedure is summarised as follows.

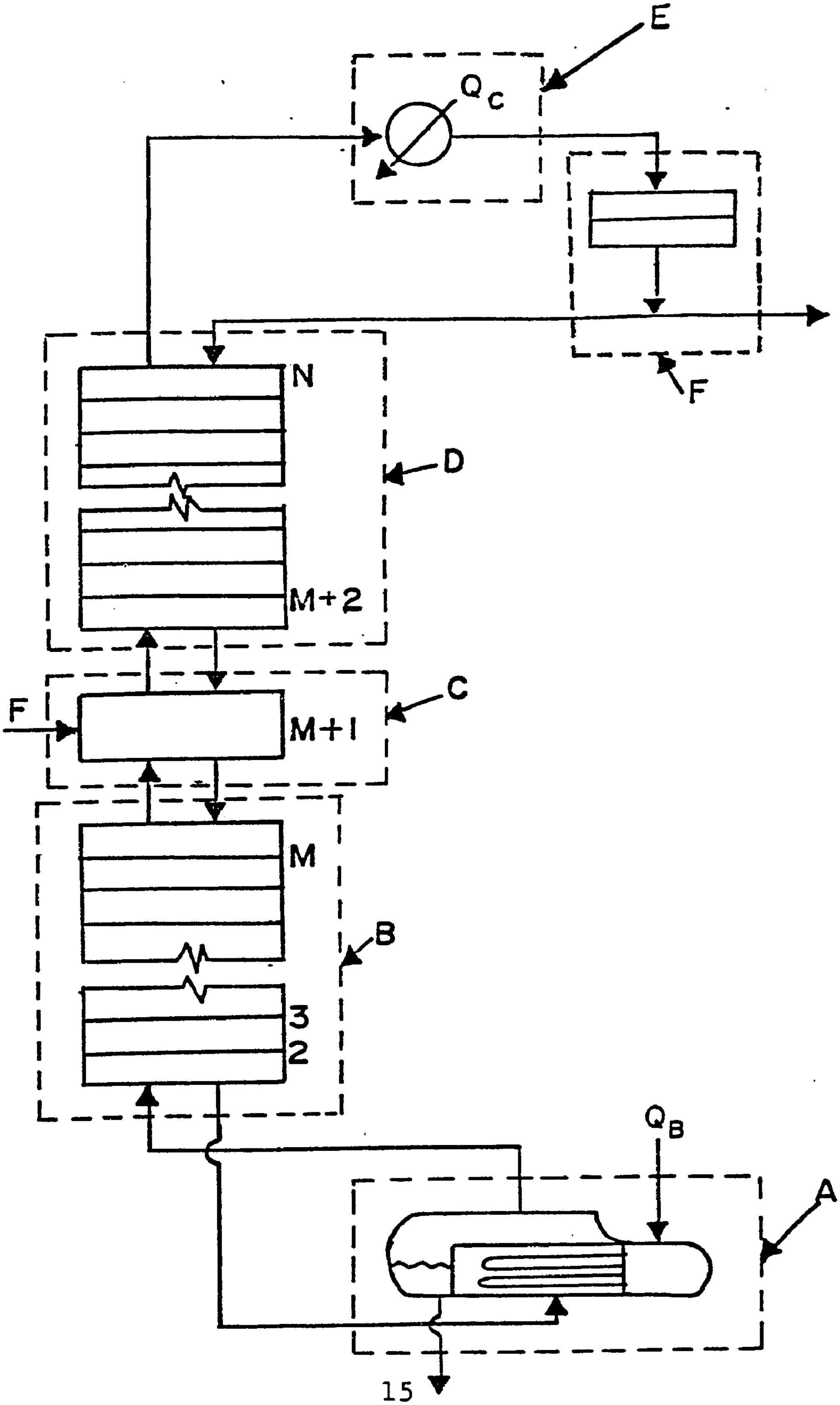
1) Select the product compositions to be controlled. For Lehigh distillation column, (binary, methanol/water, 24 tray) distillate and bottom's compositions were selected.

2) Define the process input disturbances. For the column, the input disturbances were considered to be feed composition, feed rate and feed temperature.

3) Select measurable output secondary measurements and measurable input manipulative variables. For the column, the 24 tray temperatures were considered to be easily measurable output variables. Reflux flow rate and steam flow rate were considered as measurable manipulative variables.

4) Construct the linear static model (obtain matrices R, Q, P and K). These matrices can be obtained from the steady state changes in selected output secondary measurements and product compositions for a small step change in input disturbances. This can be done experimentally or by steady state simulation of the process. For the column, the matrices were obtained by calculating steady state changes in tray temperatures and product compositions for ±1 percent changes in input disturbances and manipulative variables using a rigorous steady state model of the column.

Figure 1. Elements of a Distillation Column.



5) The minimum number of secondary measurements, say n, is equal to the number of unmeasurable input disturbances. Calculate minimax row dot product for all possible sets of n secondary measurements. The sets with minimax row dot products are candidates for use in the estimator. Out of these sets, the set with the lowest reduced model matrix condition number is selected, if the condition number is less than ten. If the condition number is greater than ten, the number of secondary measurements for use in the estimator is increased by one. The procedure is repeated, until a set of secondary measurements with acceptable condition number is found. For the column the composition estimator with three tray temperature measurements was found satisfactory.

4. RIGOROUS NONLINEAR ESTIMATORS

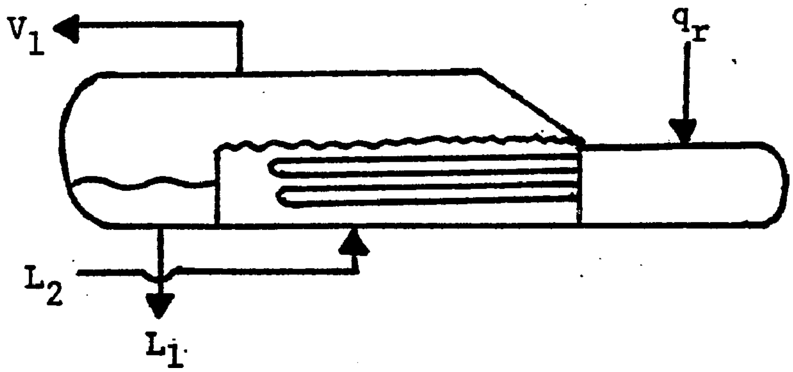
This chapter deals with steady state composition estimation for a binary distillation column based on a fundamental, nonlinear steady state model of the distillation column involving tray to tray mass and energy balances. Process flow rates and tray temperatures are considered easily measurable secondary measurements. A criterion to select an optimum subset of available secondary measurements based on sensitivity analysis is suggested. This type of estimator will be referred to as a rigorous estimator, to distinguish from estimators developed in Chapter 5.

4.1. Dimensional Analysis (14)

The degrees of freedom or the number of design variables which must be specified in any system is equal to the total number of variables in the system minus the number of restriction conditions or relationships existing in the system. An efficient approach to determine the degrees of freedom of a process unit is to break up the process unit into a number of elements and determine the degree of freedom of these elements and combine them in a proper fashion to obtain the degrees of freedom for the process unit.

Figure 1 depicts a distillation unit with one feed, total condenser and partial reboiler which has been divided into six elements, A, B, C, D, E and F.

Consider the element A, partial reboiler



A flow stream is completely specified by (C+2) variables, (C-1) for composition, temperature, pressure and flow rate.

Since three flow streams and one heat stream are involved, the total number of variables is equal to

$$N = 3(C+2) + 1 = 3C + 7$$

The restricting relationships can be tabulated as follows:

Type of Restriction	
Inherent (two equilibrium streams at the same temperature and pressure	2
Component balances	C
Overall energy balance	1
Equilibrium relationship	C
	2C+3

The degrees of freedom for element A

$$= (3C+7) - (2C+3)$$

$$= C + 4$$

In the same manner it can be shown,

Degrees of freedom for element B $= 2C + 2(M-1) + 5$

Degrees of freedom for feed stage $= 3C + 8$

Degrees of freedom for element D $= 2C + 2(N-M-1) + 5$

Degrees of freedom for element E (total condenser)

$= C + 4$

Degrees of freedom for element F $= C + 5$

The degrees of freedom of a process unit is equal to the sum of the degrees of freedom of its elements minus the restrictions imposed by bringing such units together. Since there are nine internal streams,

Number of restricting relationships $= 9 \times (C+2)$

Degrees of freedom of a distillation column

$= (10C+2N+27) - (9\times(C+2)$

$= C + 2N + 9$

In a distillation column, the following design specifications are usually available.

Pressure in each stage $= N-1$
Pressure in condenser $= 1$
Pressure in reboiler $= 1$
Pressure in reflux drum $= 1$
Heat Loss in each stage $= N-1$
Heat loss in reflux drum $= 1$
Reflux temperature $= 1$
Feed temperature $= 1$
Feed pressure $= 1$

Total number of stages = 1

Number of feed stages = 1

2N+7

Hence, additional number of variables required to specify the system completely is equal to (C+2).

The easily available tray temperature and process flow rate measurements are

$$= (N-1) + 5 = N + 4$$

The process flow rates considered are steam flow rate, feed flow rate, bottom's flow rate, reflux flow rate, and distillate flow rate. There are (N-1) available tray temperatures.

For a distillation column, if (C+2) of these (N+4) available tray temperatures and process flow rates are known, the column is completely specified.

For a binary column if four of available tray temperatures and process flow rates in any combination are known, the column is completely specified.

Similarly, for a ternary column five of these secondary measurements are necessary to define the system.

4.2 Proposed Rigorous Estimators

As mentioned earlier, for a binary distillation column if any four of the available tray temperatures and process flow rates are known, the product compositions could be estimated using a steady state mathematical model. A large number of tray temperatures and process flow rates is available.

A rigorous estimator uses a set of four or more of the available secondary measurements in conjunction with a steady state model (involving tray energy and material balances) to estimate the product qualities. A large number of combinations of sets containing at least four secondary measurements is possible. In this section, the sets of secondary measurements which are candidates to be used in rigorous estimators are proposed based on two considerations. One consideration is the ease of computations involved in product composition estimation. The second consideration is to minimize the composition estimation error due to dynamics of the column. If secondary measurements are taken from the section in which the product composition is to be controlled, the composition estimation error due to dynamics of the column may be small.

<u>RE1 Estimator</u>: In this type of rigorous estimator, the product composition is estimated by using a tray temperature and two or three process flow rates depending on the location of the tray.

The distillation column could be divided into two sections: rectifying section and stripping section. Based on the analysis of the degrees of freedom of either section, it can be shown that if three secondary measurements in a section are known, the product composition in that section could be estimated.

Distillate composition could be estimated by using reflux flow rate, distillate flow rate and a tray temperature in the rectifying section in conjunction with a steady state model for the distillation column. If a tray temperature in the stripping section is used feed flow rate, reflux flow rate and distillate flow rate measurements are required.

For bottom's product composition estimation, steam flow rate, bottom's flow rate and a tray temperature (in the stripping section) measurements are used. If a tray temperature in the rectifying section is used, additional feed flow rate measurement is also required. The computational procedures are explained in detail in Appendix B.

RE2 Estimator: A number of product composition estimates are obtained for different tray temperatures and corresponding process flow rates by the technique described in RE1 estimator.

An average of these product composition estimates is considered as the true product composition estimate.

RE3 Estimator: This estimator also uses a number of tray temperatures.

All tray temperatures in the rectifying section can be calculated for a given distillate composition if reflux flow rate and distillate flow rate measurements are available. All tray temperatures in the column can be computed for a given distillate composition if feed flow rate, reflux flow rate and distillate flow rate are known.

The distillate composition for which the sum of squares of differences between calculated tray temperatures and measured tray temperatures is minimized is considered the composition estimate.

The bottom's product composition estimate is also obtained in a similar manner. The tray temperatures in the stripping section can be calculated for a given bottom's product composition if bottom's flow rate and steam flow rate are known. To calculate all tray temperatures in the column, additional feed flow rate measurement is also required.

4.3. Sensitivity Analysis

In the previous section, the general nature of rigorous estimators was discussed. In this section, a criterion for selecting optimum tray temperatures based on sensitivity analysis is suggested.

For a steady state operation, the composition estimation error could be attributed to measurement errors (noise and sensitivity limitation of the measuring device) and to inaccuracies in the mathematical model representing the distillation column. For an RE1 estimator, a tray temperature and at most three process flow rate measurements are required. It can be written that

$$x = f(a,b,c,T_i) \tag{4}$$

where

a,b,c represent process flow rate measurements

T_i = temperature of i^{th} tray

x = product composition estimate.

It can be shown that

$$\Delta x = \frac{\partial f}{\partial a} \cdot \Delta a + \frac{\partial f}{\partial b} \cdot \Delta b + \frac{\partial f}{\partial c} \cdot \Delta c + \frac{\partial f}{\partial T_i} \cdot \Delta T_i$$

where

Δx is the composition estimation error.

$\Delta a, \Delta b, \Delta c$ and ΔT_i are measurement errors.

If the error statistics of secondary measurements are known, let $\overline{\Delta a}$, $\overline{\Delta b}$, $\overline{\Delta c}$ and $\overline{\Delta T_i}$ represent the maximum possible measurement errors. Then, the maximum composition estimation error

$$\overline{\Delta x} \leq \left|\frac{\partial f}{\partial a}\cdot\overline{\Delta a}\right|+\left|\frac{\partial f}{\partial b}\cdot\overline{\Delta b}\right|+\left|\frac{\partial f}{\partial c}\cdot\overline{\Delta c}\right|+\left|\frac{\partial f}{\partial T_i}\cdot\overline{\Delta T_i}\right|$$

$\overline{\Delta x}$ can be evaluated for each tray temperature. The tray temperature with the minimum of maximum composition estimation error is selected as an optimum tray temperature for an RE1 estimator.

For RE2 and RE3 composition estimators tray temperatures with the lowest maximum composition estimation errors are selected.

In certain cases when measurement error statistics are not available, a simpler criterion to select the optimum tray temperature is proposed. It is assumed that the maximum process flow rate measurement errors are approximately equal and that the temperature measurement error for different tray temperatures is also approximately equal. The tray temperatures for which $M_D = \{|\frac{\partial f}{\partial a}|+|\frac{\partial f}{\partial b}|+|\frac{\partial f}{\partial c}|\}$ is low are considered as candidates for optimum tray temperatures. Of these tray temperatures, one with the lowest $|\frac{\partial f}{\partial T_i}|$ is selected as an optimum tray temperature for RE1 estimator. For RE2 and RE3 estimators, the optimum tray temperatures are tray temperatures with lowest $|\frac{\partial f}{\partial T_i}|$.

Since a rigorous steady state model for the distillation column is used in the estimators, composition estimation error due to modelling errors should be small except for changes in parameter values. Composition estimation error could occur due to changes in tray efficiencies, tray pressure drops and tray heat losses. It is evident that the closer the tray temperature measurements are to the top, the smaller would be the distillate composition estimation error due to these types of variations.

For bottom's composition estimation, the lower the tray temperature measurements, the smaller the composition estimation error due to changes in tray efficiencies and tray heat losses. However, the opposite is true for composition estimation error for changes in tray pressure drops.

4.4 Sensitivity Analysis: Binary Distillation Column

In this section, steady state simulation results of sensitivity analysis for an ideal constant relative volatility, binary distillation column with equimolal overflow are described. The aim of the study was to investigate the effect of relative volatility, boiling point range of the mixture, purity of the products and tray temperature location on distillate composition estimation error due to measurement errors in reflux flow rate, distillate flow rate and tray temperature using RE1 estimator.

The binary distillation columns were optimally designed assuming reflux ratio of 1.2 times the minimum reflux ratio and optimum feed tray location. The steady state design results are described in Table 1.

To evaluate sensitivity of RE1 estimator to reflux flow rate measurement the composition estimation error was computed for ten percent error in reflux flow rate measurement assuming no measurement error in distillate flow rate and tray temperature measurements. The composition estimation error for ten percent error in distillate flow rate measurement was computed assuming no measurement error in reflux flow rate and tray temperature measurements. The composition estimation error was computed for 1°C measurement error in tray temperature measurement assuming no error in process flow rate measurements for a) when boiling range of mixture is 30°C and b) when the boiling point range of mixture is 50°C.

Figure 2 to Figure 5 represent the sensitivity plots for the ideal binary distillation columns described in Table 1. The composition estimation errors are plotted against the tray number on which temperature is measured for a) ten percent error in reflux flow rate measurement, b) ten percent error in distillate flow rate measurement, c) 1°C tray temperature measurement error when boiling point range of mixture is 30°C, and d) 1°C tray temperature measurement error when the boiling point range of mixture is 50°C. XDS represents the steady state distillate composition. ΔTB represents the boiling point range of the binary mixture. ΔXD represents the distillate composition estimation error.

Distillate composition estimation error decreased rapidly as the tray temperature measurement moved up the column for measurement error in the reflux flow rate. Composition estimation error increased as the tray temperature measurement moved up the column for measurement error in distillate flow rate. Composition estimation

Table 1. Steady State Design Results for Ideal Binary Distillation Columns

Distillate Composition (%)	Bottom's Composition (%)	Feed Composition (%)	Murphree Efficiency (%)	Relative Volatility	Number of Trays	Feed Tray Location
95	5	45	70	2.0	26	13
95	5	45	70	1.5	43	21
99	1	45	70	2.0	39	19
99	1	45	70	1.5	65	32

Figure 2. Sensitivity Analysis for Low Purity, High Relative Volatility Binary Distillation Column.

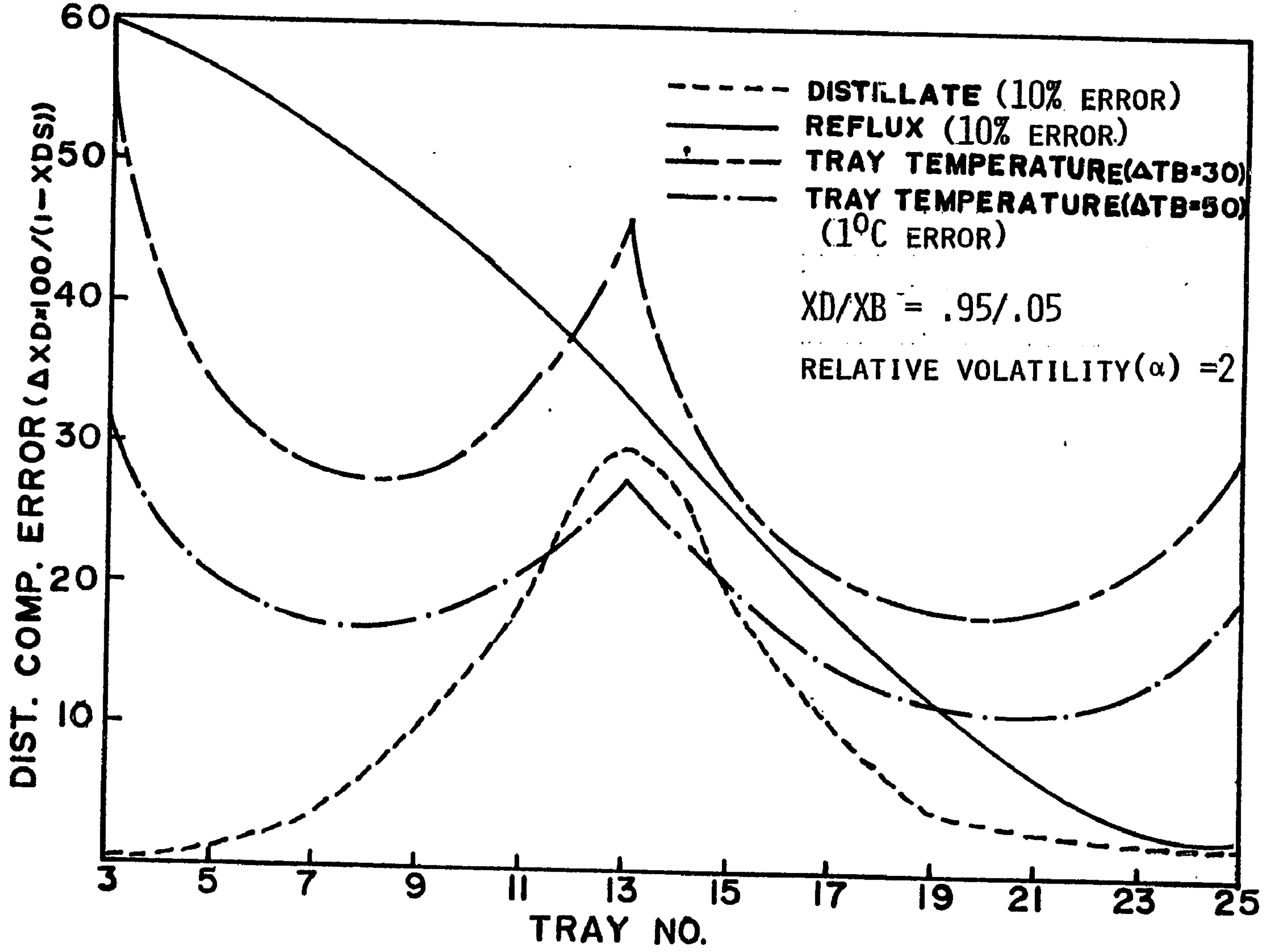


Figure 3. Sensitivity Analysis for Low Purity, Low Relative Volatility Binary Distillation Column.

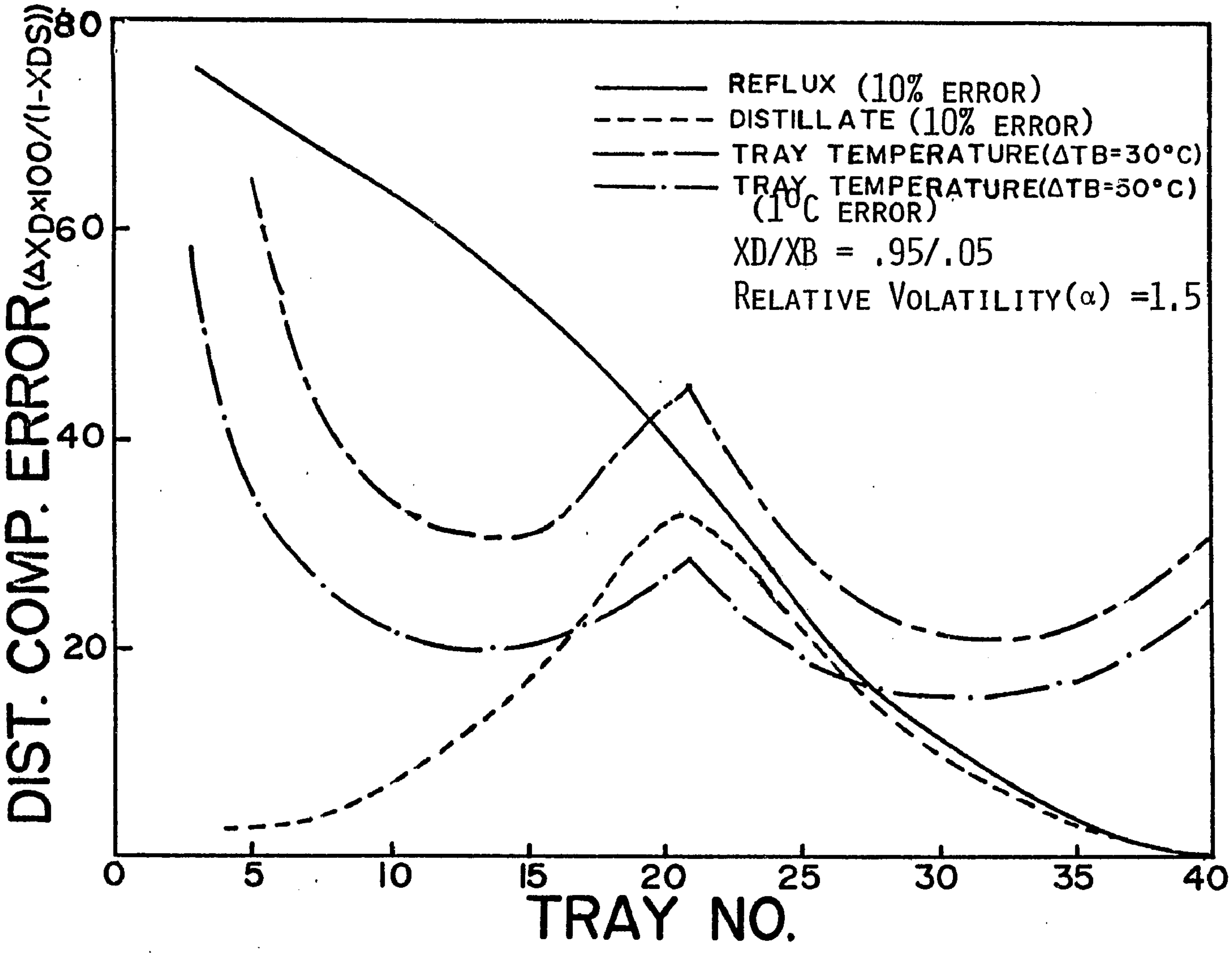


Figure 4. Sensitivity Analysis for High Purity, High Relative Volatility Binary Distillation Column.

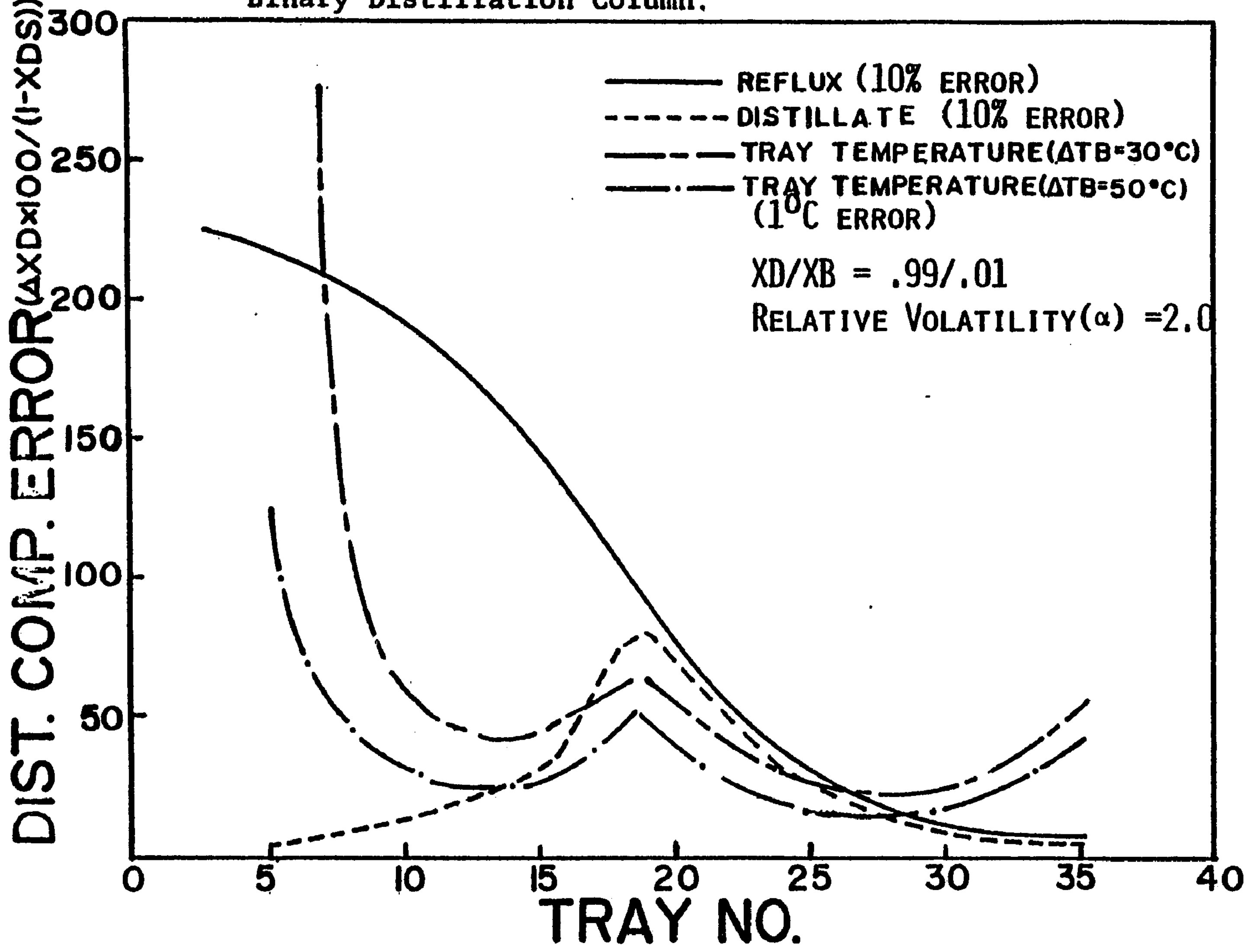
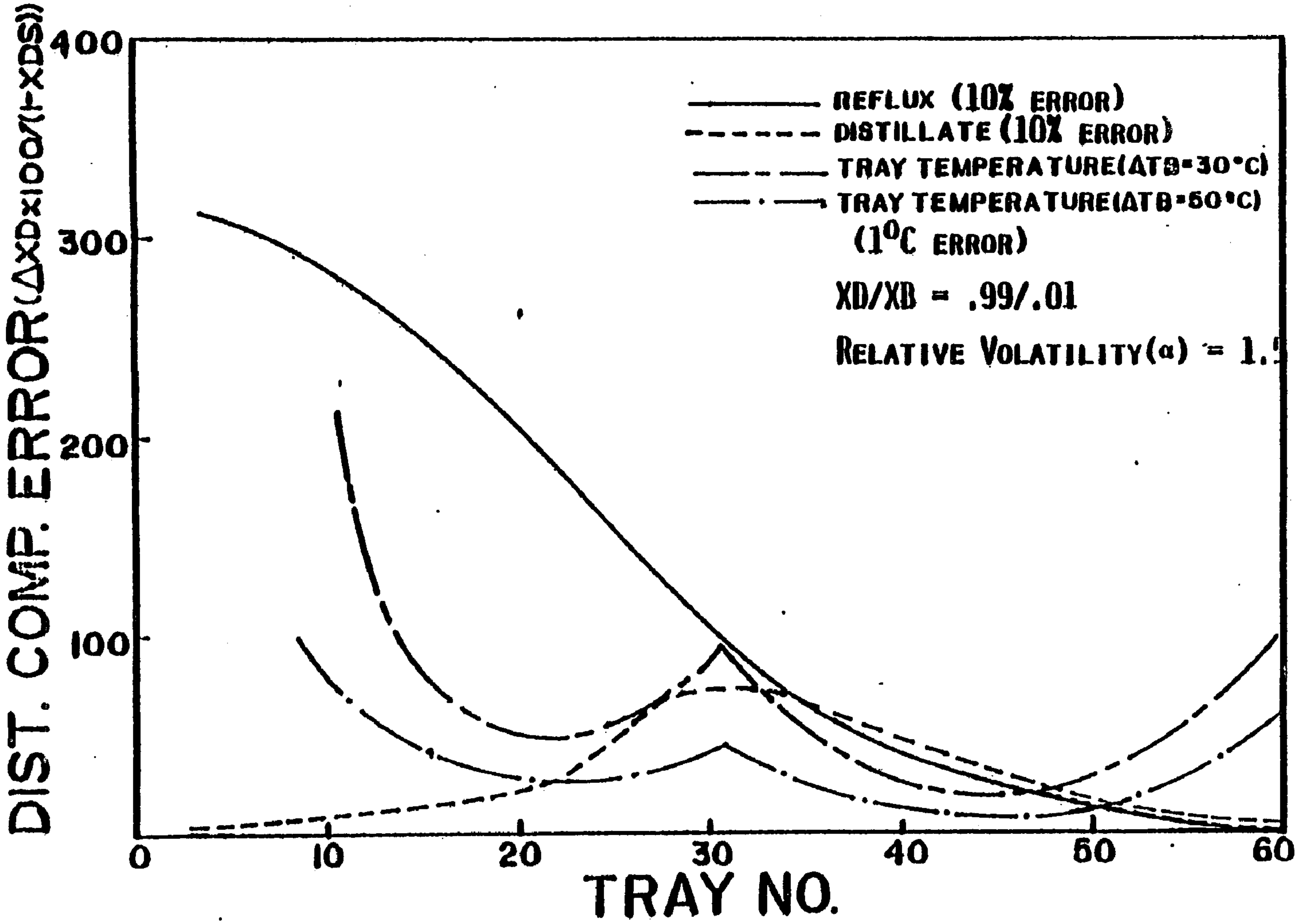


Figure 5. Sensitivity Analysis for High Purity, Low Relative Volatility Binary Distillation Column.



error decreased as tray temperature measurement location moved up the column in the bottom's section, passed through a mimimum in the middle of stripping section and reached a maximum near feed tray, began to decline as tray temperature measurement moved up in the rectifying section, passed through a minimum and again increased rapidly for tray temperature measurement error.

The composition estimation errors were smaller for the low purity distillation column. The composition estimation errors were smaller for low relative volatility mixtures for measurement errors in distillate flow rate and tray temperatures, while the opposite was true for measurement error in reflux flow rate. The composition estimation error due to tray temperature measurement error were smaller for mixtures with large boiling point range.

The optimum tray measurement location for RE1 estimator to control distillate composition should lie somewhere in the middle of the rectifying section.

5. APPROXIMATE NONLINEAR ESTIMATORS

The estimators proposed in this section are referred to as approximate estimators to distinguish them from other types of estimators.

These estimators are designed for a binary distillation column with one feed stream and no side streams. Indirect composition control is achieved by controlling ϕ, a newly defined quantity which is function of process flow rates (reflux and/or steam flow rate) and/or tray temperatures by manipulating reflux and/or steam flow rate. In design of these estimators process nonlinearities in face of feed composition disturbances are taken into consideration. In this aspect, they are superior to Brosilow's linear estimator. These estimators can be designed using a rigorous steady state model for the distillation column or by using the steady state operating data of the distillation column. One serious limitation of these estimators is that it is not possible to give composition set point changes. The product compositions can only be maintained on the target value for which they are designed.

5.1. Proposed Approximate Estimators

For a binary distillation column, the system is completely specified if four system variables are fixed.

When the control objective is to maintain desired distillate composition, the steam flow rate to the reboiler is maintained constant. The reboiler heat load is fixed. The distillate composition is also fixed. If the volumetric feed rate is assumed constant, then for a given feed composition the column is completely specified. For a given feed composition, the tray temperatures and process flow rates assume unique values.

There is a functional relationship between tray temperatures and reflux flow rate. Using a rigorous steady state model of the distillation column, a number of sets of values of tray temperatures and corresponding reflux flow rate can be computed for different feed compositions. Alternatively, these sets of values of tray temperatures and corresponding reflux flow rate can be obtained experimentally by operating column at steady state for different feed compositions.

AE 1 Estimator: As mentioned, each tray temperature is a single valued function of reflux flow rate. The temperature of i^{th} tray can be expressed as a n^{th} order polynomial function of reflux flow rate using least square criterion as described in Eq. (1). The order of the polynomial depends on the desired accuracy.

$$T_i^c = \sum_{m=1}^{n} A(i,m) \times R^{(m-1)} \qquad (1)$$

where

T_i^c represents the calculated temperature of i^{th} tray

R is the reflux flow rate.

Distillate composition is controlled by manipulating reflux flow rate. If the reflux flow rate is maintained such that the temperature of i^{th} tray is equal to the calculated temperature of i^{th} tray, no steady state composition error would occur in face of feed composition disturbances. A new quantity, say $\phi 1$, which is difference of calculated temperature of i^{th} tray and actual temperature of i^{th} tray is defined. Distillate composition control can be achieved by manipulating reflux flow rate such that $\phi 1$ is maintained on the target value of zero.

$$\phi 1 = T_i^c - T_i = \sum_{m=1}^{n} A(i,m) \times R^{(m-1)} - T_i \qquad (2)$$

<u>AE2 Estimator</u>: Each tray temperature is a single valued function of reflux flow rate. Conversely, it is also true that reflux flow rate can be expressed as a function of any tray temperature. The reflux flow rate can be expressed as a n^{th} order polynomial function of temperature of i^{th} tray using least square criterion as described in Eq. (3). The order of the polynomial depends on the desired accuracy.

$$R_i^c = \sum_{m=1}^{n} B(i,m) \times (T_i)^{(m-1)} \qquad (3)$$

Let $\phi 2$ be defined as a difference between calculated value of reflux flow rate using i^{th} tray temperature and actual reflux flow rate.

$$\phi 2 = R_i^c - R = \sum_{m=1}^{n} B(i,m) \times (T_i)^{m-1} - R \qquad (4)$$

Composition control can be achieved by manipulating reflux flow rate such that R_i^c is maintained equal to reflux flow rate. Alternatively, distillation composition control can be achieved by manipulating reflux flow rate such that $\phi 2$ is maintained on the target value of zero.

<u>AE3 Estimator</u>: From Eq. (3),

$R_i^c = \sum_{m=1}^{n} B(i,m) \times (T_i)^{m-1}$ where T_i is the tray temperature of i^{th} tray.

It can also be shown,

$R_j^c = \sum_{m=1}^{n} B(j,m) \times (T_j)^{m-1}$ where T_j is the tray temperature of j^{th} tray.

At steady state, if distillation composition is maintained constant, R_i^c and R_j^c should equal actual reflux flow rate in face of feed composition disturbances.

Let $\phi 3$ be defined as difference between R_i^c and R_j^c.

The distillate composition control can be achieved by manipulating reflux flow rate such that $\phi 3$ is maintained on the target value of zero.

$$\phi 3 = R_i^c - R_i^c$$

$$= \sum_{m=1}^{n} B(i,m) \times (T_i)^{(m-1)} - \sum_{m=1}^{n} B(j,m) \times (T_j)^{(m-1)} \qquad (5)$$

AE4 Estimator: Assume that the tray temperatures are expressed as a third order polynomial of reflux flow rate to achieve desired accuracy. The steady state values of temperatures of i^{th}, j^{th}, k^{th} and th tray are available.

From Eq. (1)

$$T_i^c = \sum_{m=1}^{4} A(i,m) \cdot R^{(m-1)} \qquad (6)$$

Since at steady state $T_i^c \simeq T_i$, using Eq. (6)

$$T_i = \sum_{m=1}^{4} A(i,m) \cdot R^{(m-1)} \qquad (7)$$

Similarly,

$$T_j = \sum_{m=1}^{4} A(j,m) \cdot R^{(m-1)} \qquad (8)$$

$$T_k = \sum_{m=1}^{4} A(k,m) \cdot R^{(m-1)} \qquad (9)$$

$$T_\ell = \sum_{m=1}^{4} A(\ell,m) \cdot R^{(m-1)} \qquad (10)$$

Using Eq. (7), Eq. (8), and Eq. (9), it can be shown

$$\{\tilde{T}\} = \{\tilde{A}\}\{\tilde{R}\} \qquad (11)$$

where

$$\{\tilde{T}\} = \begin{Bmatrix} T_i - A(i,1) \\ T_j - A(j,1) \\ T_k - A(k,1) \end{Bmatrix} ; \{A\} = \begin{Bmatrix} A(i,2) A(i,3) A(i,4) \\ A(j,2) A(j,3) A(j,4) \\ A(k,2) A(k,3) A(k,4) \end{Bmatrix} ; \{\tilde{R}\} = \begin{Bmatrix} R \\ R^2 \\ R^3 \end{Bmatrix}$$

Eq. (10) can be expressed in the matrix form as

$$T_\ell = A(\ell,1) + \{A1\}\{\tilde{R}\} \qquad (12)$$

where $\{\tilde{A1}\}$ is a raw matrix $A(\ell,2), A(\ell,3) A(\ell,4)$.

From Eq. (11),

$$\{\tilde{R}\} = \{\tilde{A}\}^{-1}\{\tilde{T}\} \tag{13}$$

Substituting for $\{\tilde{R}\}$ from Eq. (13) in Eq. (12)

$$T_\ell = A(\ell,1) + \{\tilde{A1}\}\{\tilde{A}\}^{-1}\{\tilde{T}\} \tag{14}$$

Eq. (14) can be expressed as follows, after matrix multiplication

$$T_\ell = C1 + C2T_i + C3T_j + C4T_k \tag{15}$$

Distillation composition control can be achieved if reflux flow rate is manipulated such that the relationship between the tray temperatures as expressed in Eq. (15) is maintained.

A new quantity $\phi4$ is defined as follows.

$$\phi4 = T_\ell - C1 - C2T_i - C3T_j - C4T_k \tag{16}$$

Distillate composition control can be achieved by manipulating reflux flow rate such that $\phi4$ is maintained on the target value of zero.

If tray temperature can be expressed as n^{th} order polynomial of reflux flow rate for desired accuracy, then $\phi4$ would be a linear function of (n+1) tray temperatures.

In design of these estimators it was assumed that the volumetric feed rate is constant. In case of AE1 and AE2 estimator, if $R' = \frac{R \times F_o}{F}$ is substituted for R in the equations defining ϕ, the composition control can be maintained in face of feed rate disturbances. F is the volumetric feed rate at a given time and F_o is the volumetric flow rate for which the estimators are designed. In case of AE3 and AE4 estimators, since ϕ is only a function of tray temperatures, composition control can be accomplished without modifying the definition of ϕ in face of feed rate disturbances.

Generally, when the control objective is to maintain bottom's product composition, reflux flow rate is maintained constant. Following the logic applied in developing distillate composition approximate estimators, each tray temperature can be expressed as a polynomial function of steam flow rate using least square criterion. The approximate estimators of similar type can be developed. ϕ would be a function of steam flow rate and/or tray temperatures. The bottom's product composition is controlled by manipulating steam flow rate such that ϕ is maintained on the target value of zero.

For dual composition control, the distillate composition is controlled by manipulating reflux flow rate and the bottom's composition is controlled by maniuplating steam flow rate. However, the desired distillate composition and bottom's product composition are fixed. If the feed flow rate is constant, then for a given feed composition, the tray temperatures and process flow rates assume unique value. A number of sets of values of tray temperatures, corresponding steam flow rate and reflux flow rate can be computed using a steady state model for different feed compositions. The tray temperatures are single-valued functions of reflux flow rate. Also, the steam flow rate is a single valued function of reflux flow rate. The tray temperatures can be expressed as n^{th} order polynomials of reflux flow rate by using least square criterion. Similarly, steam flow rate can also be expressed as a polynomial function of reflux rate, as shown in Eq. (17)

$$S.F. = \sum_{i=1}^{m} C(i) \times R^{(i-1)} \tag{17}$$

The same type of approximate estimators as developed for distillate composition control are proposed for dual composition control. ϕ is a function of reflux rate and/or tray temperatures. The dual composition control is achieved by manipulating reflux rate such that ϕ is maintained on the target value of zero. However, steam flow rate is also manipulated as a function of reflux rate as described in the Eq. (17) at the same time.

Table 2 summarizes various approximate estimators proposed for distillation composition control.

5.2. Selection of Measurements

In this section, a criterion to select optimum tray temperature measurements for approximate estimators is developed.

The optimum tray temperatures are selected such that

Table 2. Description of Proposed Approximate Estimators for Distillate Composition Control.

Designation	Control Variable	Manipulative Variable	Equation	Measured Variables
AE1 Estimator, n^{th} order	ϕ_1	R	$\phi_1 = \sum_{m=1}^{n+1} A(i,m)\, R^{m-1} - T_i$	R, T_i
AE2 Estimator n^{th} order	ϕ_2	R	$\phi_2 = \sum_{m=1}^{n+1} B(i,m)\, T_i^{m-1} - R$	R, T_i
AE3 Estimator, n^{th} order	ϕ_2	R	$\phi_3 = \sum_{m=1}^{n+1} B(i,m) T_i^{m-1} - \sum_{m=1}^{n+1} G(j,m) T_j^{m-1}$	T_i, T_j
AE4 Estimator, n^{th} order	ϕ_3	R	$\phi_4 = C_o + \sum_{m=1}^{n+1} C_m T_m$	$T_1 \ldots T_m$

R = Reflux flow rate

T_i = Temperature of i^{th} tray

the steady state composition error due to measurement errors in process flow rates or tray temperatures is minimized. Let $|\Delta\phi|$ be the maximum error due to measurement errors in process flow rates or tray temperatures. For example, in case of AE1 estimator for distillate composition control

$$\phi 1 = T_i^c - T_i = f(R) = T_i$$

If ΔR and ΔT_i are maximum possible measurement errors in reflux flow rate and tray temperature of i^{th} tray

$$|\Delta\phi 1| \leq \left|\frac{dT_i^c}{dR} \cdot \Delta R\right| + |\Delta T_i| \tag{18}$$

Similarly for AE2 estimator for distillate composition control,

$$|\Delta\phi 2| \leq \left|\frac{dR_i^c}{dT_i} \cdot \Delta T_i\right| + |\Delta R| \tag{19}$$

Similarly for AE3 estimator for distillate composition control

$$|\Delta\phi 3| \leq \left|\frac{dR_i^c}{dT_i} \cdot \Delta T_i\right| + \left|\frac{dR_i^c}{dT_j} \cdot \Delta T_j\right| \tag{20}$$

Similarly for AE4 estimator

$$|\Delta\phi 4| \leq |\Delta T_\ell| + |C2 \cdot \Delta T_i| + |C3 \cdot \Delta T_j| + |C4 \cdot \Delta T_k| \tag{21}$$

By using a steady state model, the sensitivity of product composition to changes in the value of ϕ can be computed.

Let $a = \frac{\Delta x}{\Delta\phi}$ (22)

Δx is the change in product composition

$\Delta\phi$ is the corresponding change in the value of ϕ.

The maximum steady state composition error $|\Delta x_m|$ is

$$|\Delta x_m| \leq a \cdot |\Delta\phi| \qquad (23)$$

The set of tray temperatures for which $|\Delta x_m|$ is lowest is considered optimum set of tray temperatures for approximate estimators.

6. STEADY STATE SIMULATION

One aim of present research was to study the applicability of control schemes using nonlinear estimators and compare them with composition control strategies using Brosilow's linear estimator and conventional control techniques. The first logical step would be to compare steady state composition errors associated with the composition estimators and conventional control techniques in face of feed composition and/or product composition set point changes. It would be necessary to develop a rigorous steady state program for the column.

6.1 Steady State Model

The steady state model involves tray to tray mass and energy balances. It is based on the following assumptions.

1) Perfect tray mixing.
2) Perfect mixing in reflux drum and reboiler.
3) Constant tray heat losses.
4) Constant tray efficiency in rectifying section, and in stripping section.
5) Constant tray pressure drop throughout the column.

Experimental steady state data from the 24-tray column was obtained by putting steam flow rate and reflux flow rate on automatic flow control. The product compositions and feed composition were determined by withdrawing samples from the respective lines after cooling below 15°C to avoid flashing.

The recorded flow rates were adjusted slightly to make them consistent with the overall material balance for the system. The heat losses were calculated by overall energy balance around the system.

To determine tray efficiencies in the rectifying and stripping sections, it was assumed that measured compositions and adjusted process flow rates were correct. Then a set of tray efficiences in the rectifying and stripping sections were calculated such that ψ was minimized. ψ was defined as the summation of squares of differences between 6 recorded tray temperatures and calculated tray temperatures. The procedure was as follows.

1) The stripping section tray efficiency was assumed.
2) The rectifying section tray efficiency was calculated such that for a given reflux flow rate, the distillate composition calculated using the steady state model is equal to the recorded distillate composition.
3) The above procedure was repeated for different values of stripping section efficiency to minimize the value of ψ using interval halving convergence method.
4) This was continued until the set of efficiencies which minimizes the value of ψ was found.

Two steady state operating conditions were used. The first steady state was for higher feed composition. This data was used for simulation studies on distillate composition and dual composition control.

The second steady state was at lower feed composition to achieve high purity bottom's product. This was used for simulation studies on bottom's composition control.

Average operating data for both these steady states and a detailed material and energy balance for steady state No. 2 is described in Appendix C.

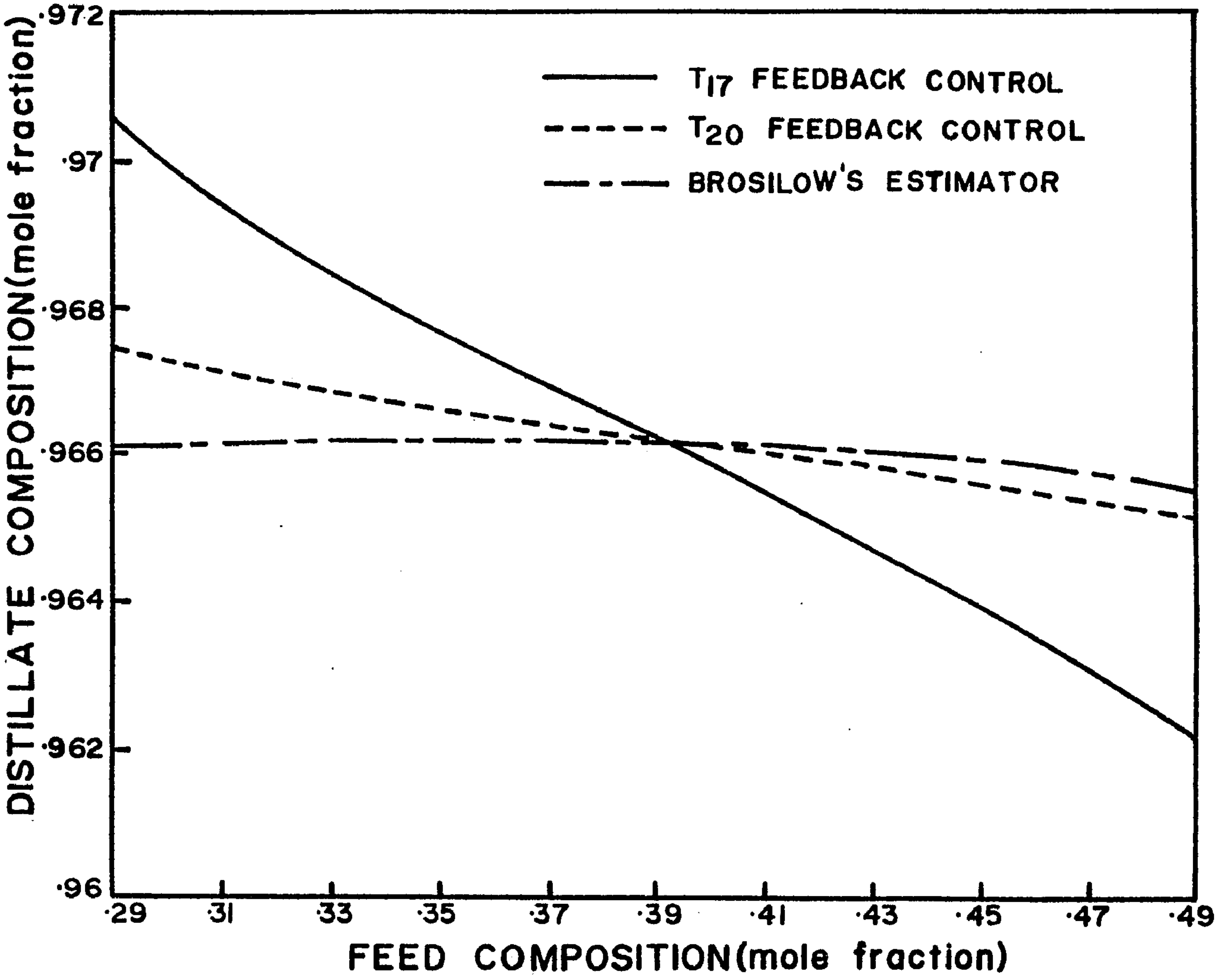
6.2. Steady State Composition Error for Constant Tray Temperature Control

For many industrial columns the indirect composition control is achieved by controlling a tray temperature near the end where the product is withdrawn.

Thus, distillate composition control is achieved by controlling a tray temperature in the rectifying section. Bottom's composition control is achieved by controlling a tray temperature in the stripping section and dual composition control is accomplished by controlling two tray temperatures, one in each section of the column.

Figure 6 shows the steady state distillate composition error when temperatures of tray 17 and tray 20 are controlled in face of changes in feed composition. The higher the control tray location, the smaller the steady

Figure 6. Steady State Distillate Composition Error for Constant Tray Temperature Control and Brosilow's Linear Estimator for Changes in Feed Composition.



state composition error.

The steady state bottom's composition error is shown in Figure 7 for different control tray locations for changes in feed composition. The lower the control tray location, the smaller the steady state composition error.

Figure 8 and Figure 9 show the steady state product composition errors when two tray temperatures are controlled simultaneously (dual composition control) for feed composition changes. For the same control tray temperature in the rectifying section, the lower the control tray temperature location in the stripping section, the smaller the steady state bottom's product composition error and the larger the steady state distillate composition error for changes in feed composition.

This study would suggest that the tray temperature closest to the end where the product is withdrawn be selected as control tray temperatures, theoretically. In practice, these trays would register small temperature changes for product composition changes (especially for high purity columns) which are difficult to detect because of sensitivity limitation of temperature sensors. A trade-off would be necessary.

Tray 17 is selected as a control tray for distillate composition control. Tray 4 is selected as a control tray for bottom's composition control. Tray 17 and Tray 4 are selected as control trays for dual composition control.

Figure 7. Steady State Bottom's Product Composition Error for Constant Tray Temperature Control and Brosilow's Linear Estimator for Changes in Feed Composition.

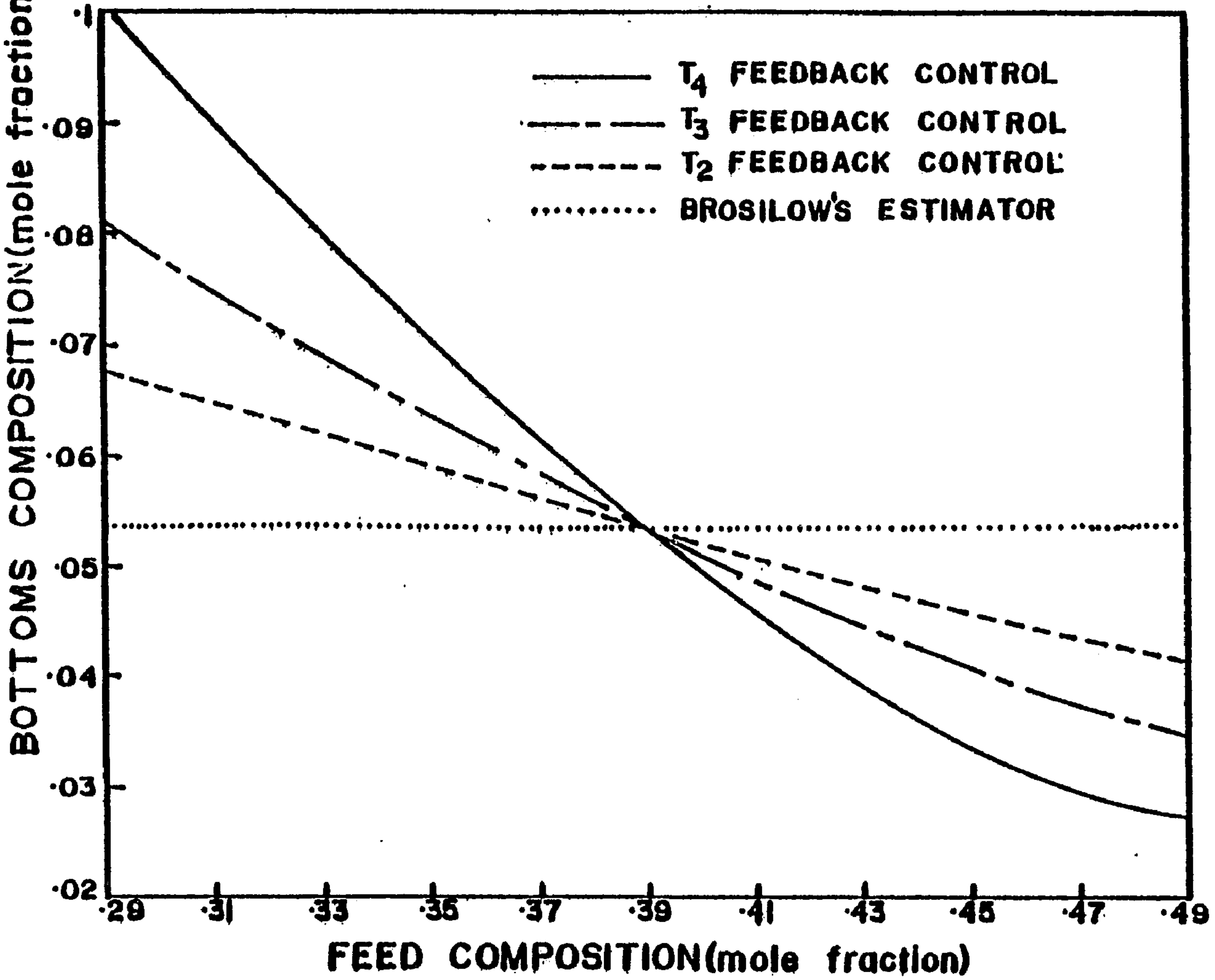


Figure 8. Steady State Distillate Composition Error for Constant Tray Temperature Control and Brosilow's Linear Estimator for Changes in Feed Composition (Dual Composition Control).

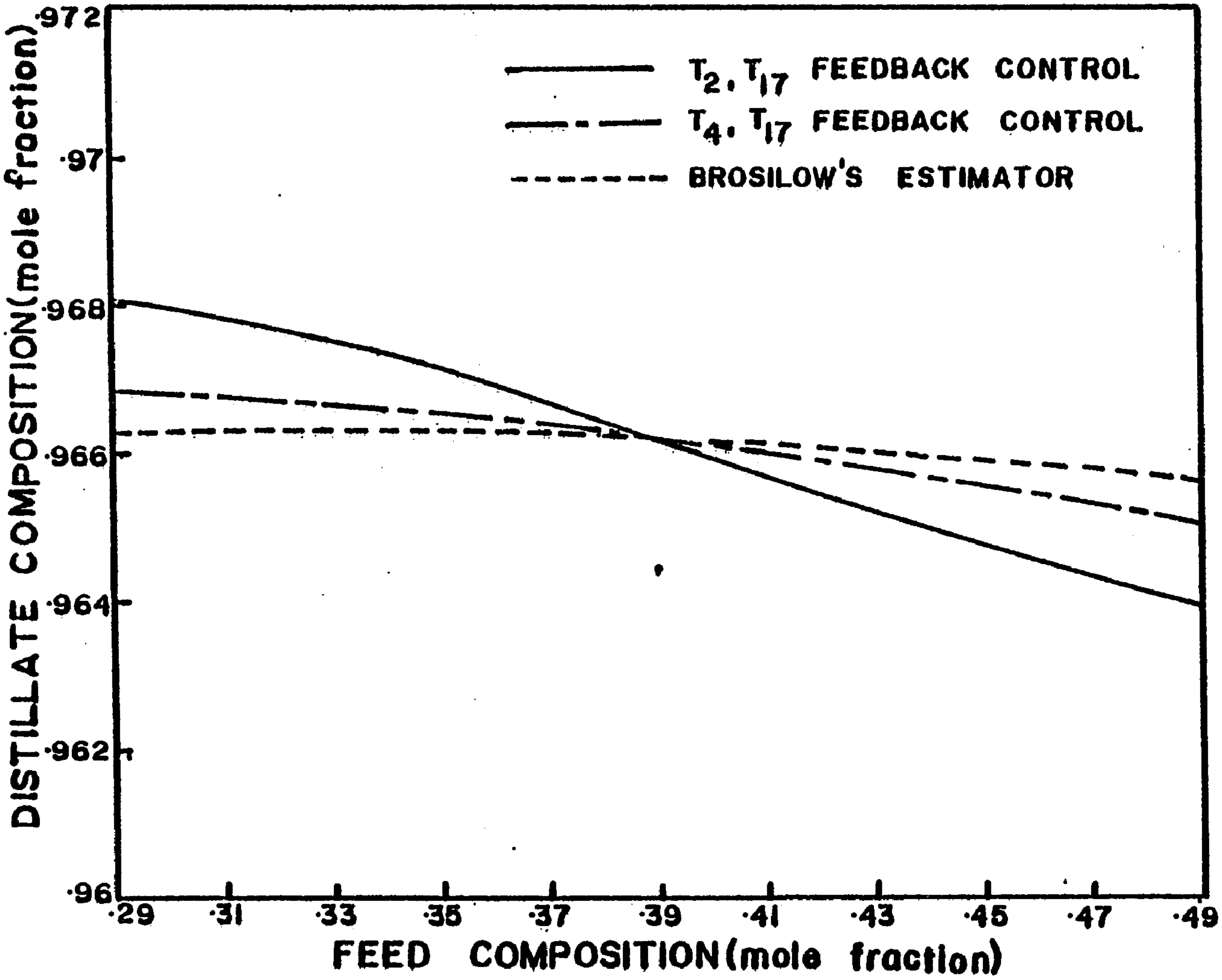
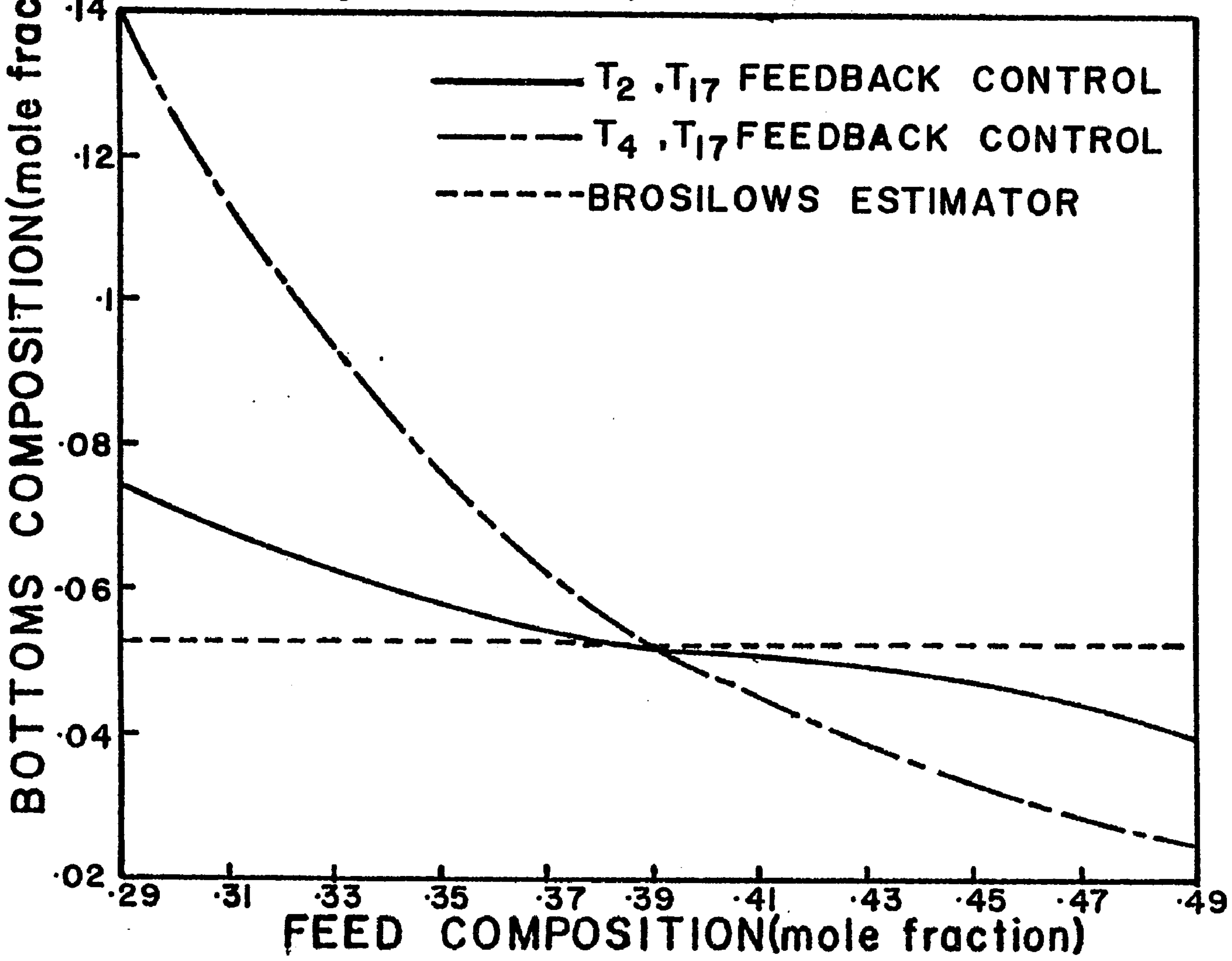


Figure 9. Steady State Bottom's Composition Error for Constant Tray Temperature Control and Brosilow's Linear Estimator for Changes in Feed Composition (Dual Composition Control).



6.3. Steady State Composition Error for Brosilow's Linear Estimator

To design the Brosilow's linear estimator, the first step was to generate a linear steady state model by perturbation techniques. The input disturbances were taken to be feed flow rate, feed temperature, feed composition, reflux flow and steam flow rate. Feed composition, feed flow and feed temperature were considered to be unmeasurable input disturbances. Although, in practice, the feed flow rate and feed temperature could be easily measured, the estimator designed on such an assumption would involve only one tray temperature measurement. For the sake of comparison with other estimators, an estimator using multiple tray temperatures was perceived as desirable. To obtain a unique Brosilow's linear estimator (not dependent on the units of secondary measurements), the input disturbances were represented in a dimensionless form (the perturbation in the value of input variable divided the steady state value of the input variable used in constructing the estimator). Tray temperatures were taken to be measurable output perturbations. The product compositions were considered unmeasurable output perturbations to be controlled. To obtain the linear static model, the steady state changes in tray temperatures and product compositions were calculated for ±1 percent change in input disturbances using a rigorous steady state model for the column.

Table 3 lists the Brosilow's linear estimators constructed to estimate the product compositions (the design technique described in Chapter 3). These estimators used three optimum tray temperatures. (The word "optimum" is used in the sense of minimizing the projection error.)

Figure 6 and Figure 12 shows steady state distillate composition error for Brosilow's linear estimator (steady state No. 1) for changes in feed composition. The control objective was to control the distillate composition. Figure 10 shows the composition error for changes in distillate composition set points.

Figure.7 shows steady state bottom's product composition error for Brosilow's estimator (steady state No. 2) for changes in feed composition. The control objective was to maintain bottom's product composition. Figure 11 shows the composition error for changes in bottom's product composition set points.

Figure 8, Figure 9, Figure 14 and Figure 16 show product composition errors for Brosilow's estimator (steady state No. 1) for changes in feed composition. The control objective was dual composition control.

The steady state composition errors for changes in feed composition are negligibly small in all three cases. The steady state distillate composition error for changes in distillate composition set points is also very small.

Figure 10. Steady State Distillate Composition Error for Brosilow's Estimator for Changes in Distillation Composition Setpoints.

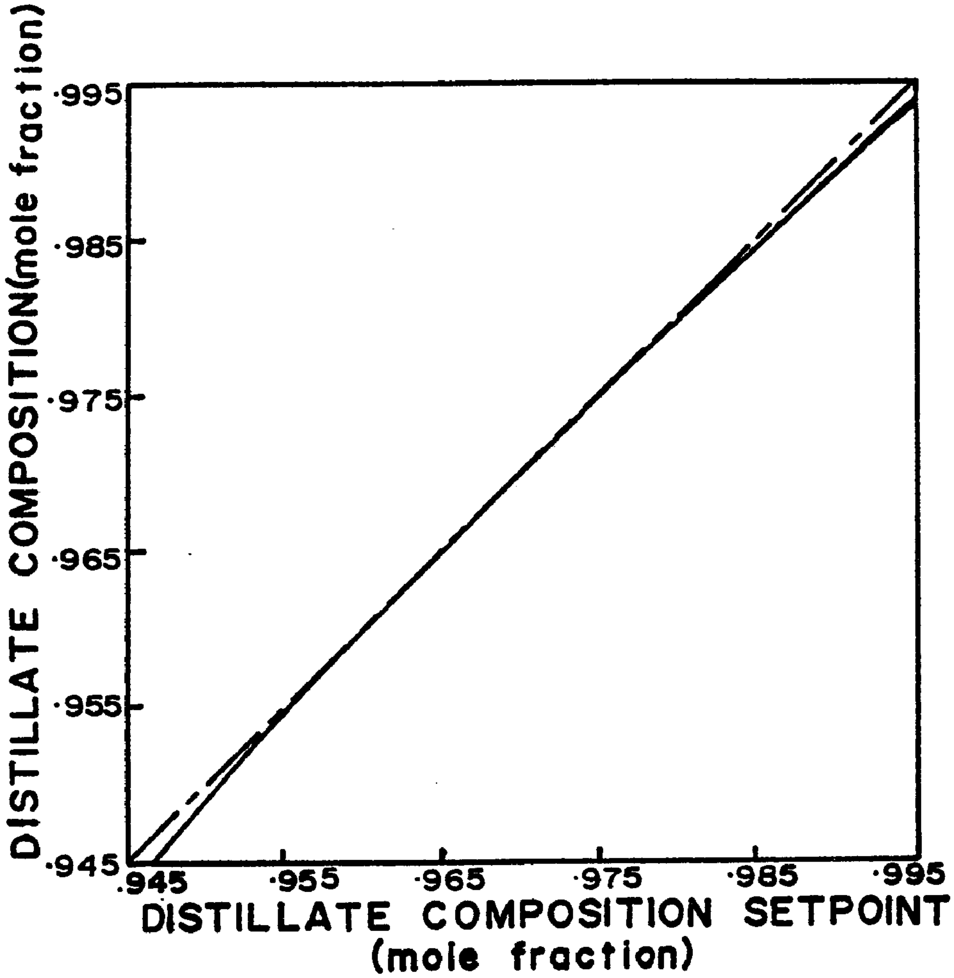


Figure 11. Steady State Bottom's Composition Error for Brosilow's Estimator for Changes in Bottom's Composition Setpoints.

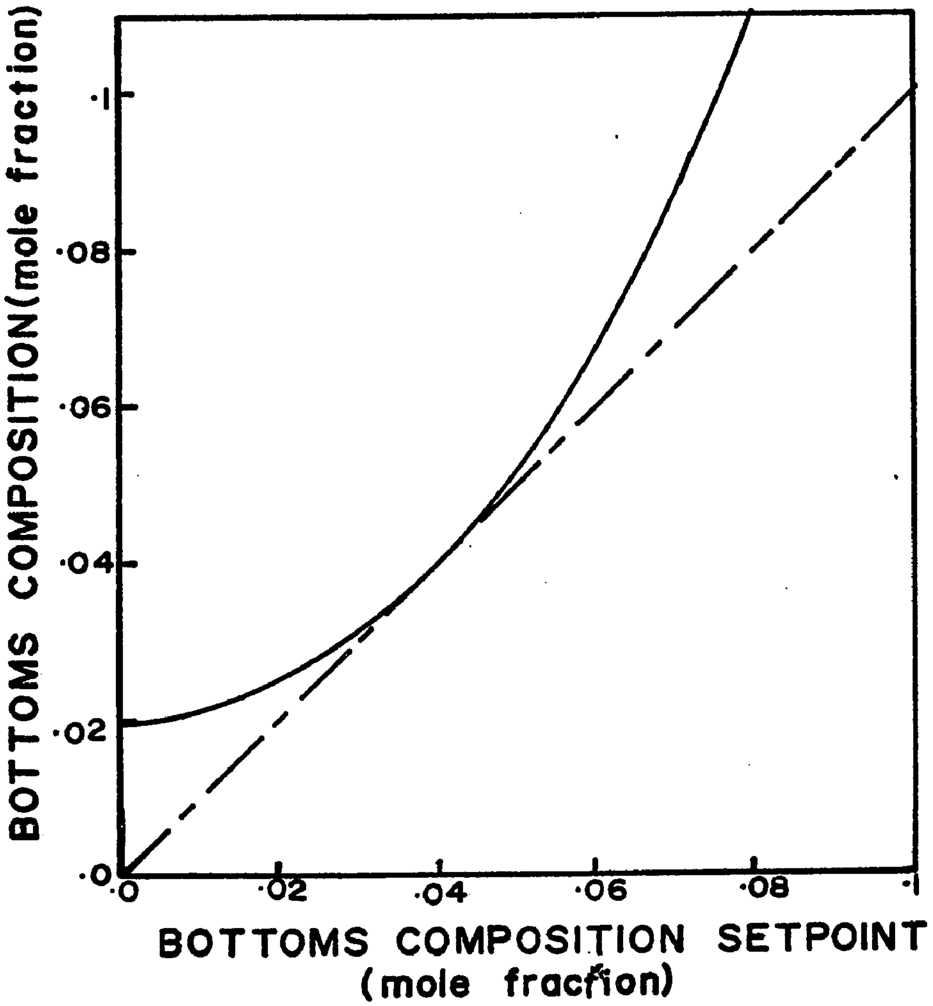


Figure 12. Steady State Distillate Composition Error for AE1 Estimator and Brosilow's Estimator for Feed Composition Changes.

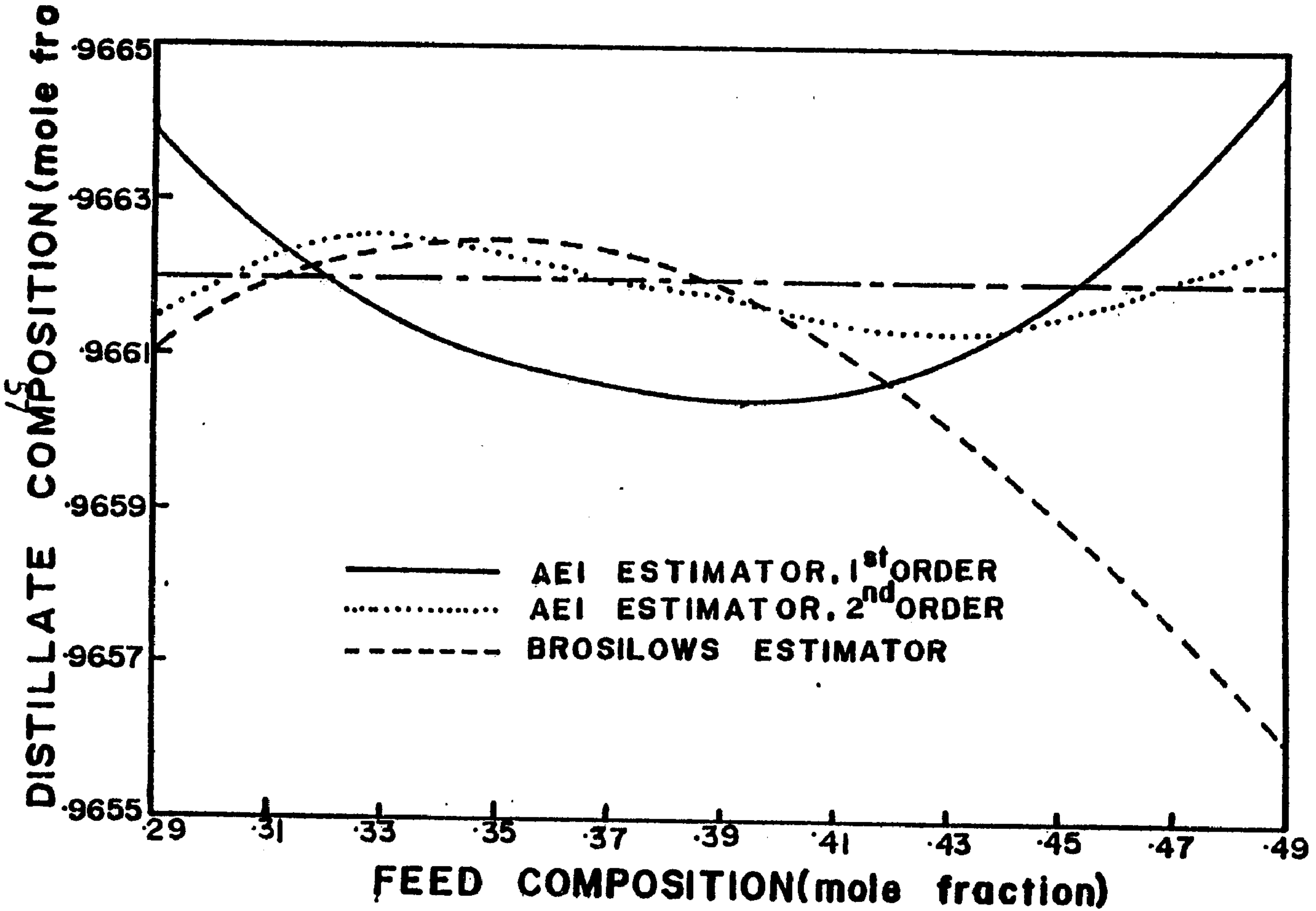


Figure 13. Steady State Distillate Composition Error for AE3 and AE4 Estimators for Changes in Feed Composition

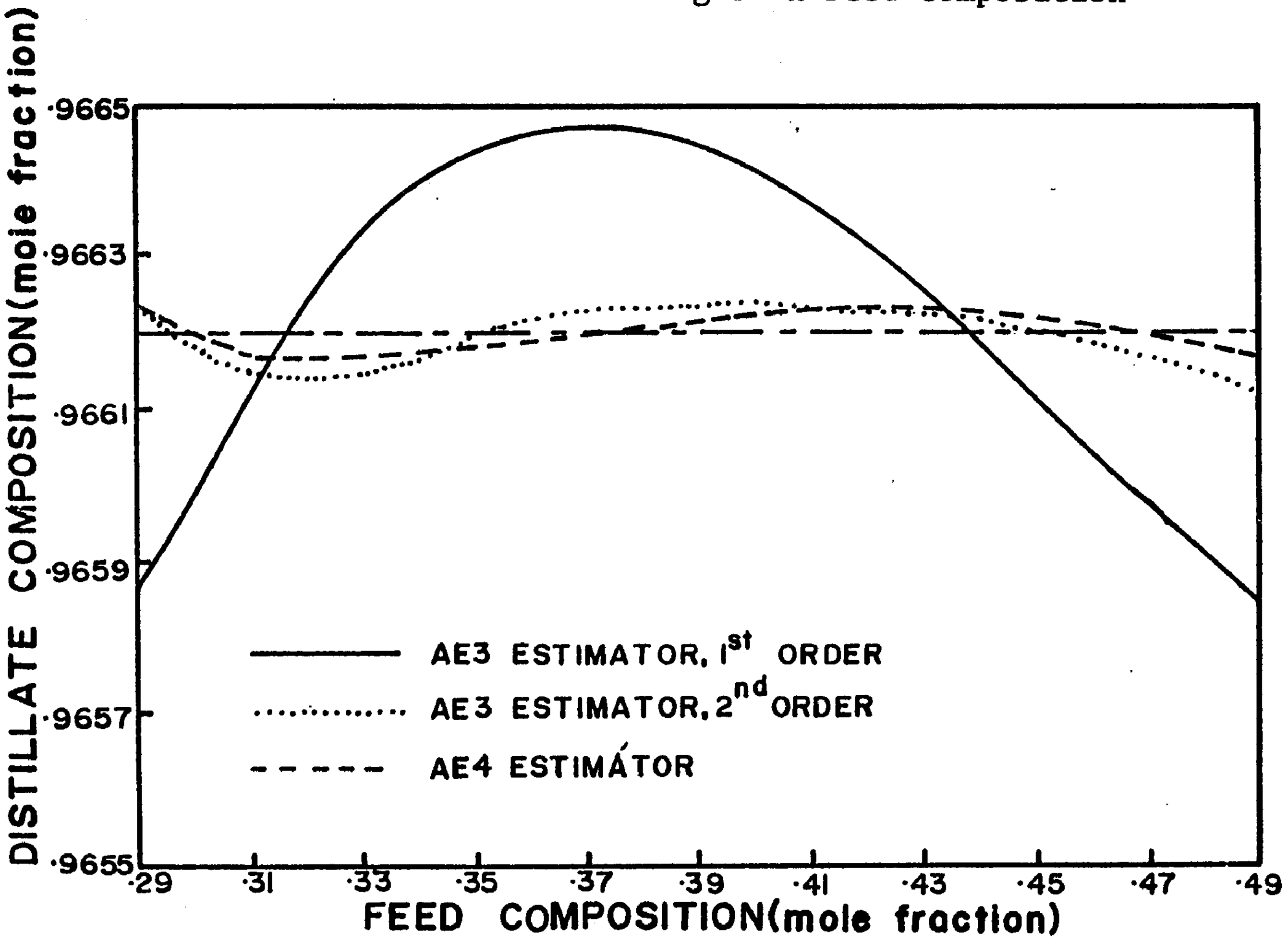


Table 3. Brosilow's Linear Estimators

STEADY STATE NO. 1

$$\Delta xD = -.0000335\ \Delta R' + .0019822\ \Delta S' + .0000223\ \Delta T_1 + .0020776\ \Delta T_9 - .010059\ \Delta T_{16}$$

$$\Delta xB = .0117787\ \Delta R' - .0101007\ \Delta S' - .0116693\ \Delta T_1 + .0048860\ \Delta T_9 - .0016796\ \Delta T_{16}$$

STEADY STATE NO. 2

$$\Delta xD = -.0003909\ \Delta R' + .0010849\ \Delta S' + .0003982\ \Delta T_5 + .0004473\ \Delta T_8 - .0077345\ \Delta T_{17}$$

$$\Delta xB = .02119\ \Delta R' - .0171243\ \Delta S' - .0423849\ \Delta T_5 + .0387318\ \Delta T_8 + .0011154\ \Delta T_{17}$$

$\Delta R'$ - Ratio of change in reflux flow rate divided by steady state value of reflux flow rate.

$\Delta S'$ - Ratio of change in steam rate divided by steady state value of steam rate.

However, the steady state bottom's product composition error is significant for changes in bottom's product composition set points when using Brosilow's estimator.

6.4. Steady State Composition Error for Approximate Estimators

To construct approximate estimators for distillate composition control, sets of values of column tray temperatures and corresponding reflux flow rate were obtained for feed composition changes from -10 to +10 percent in steps of 2 percent. Then the tray temperatures were expressed as a polynomial function of reflux flow rate (as described in Chapter 5) using least square criterion.

Table 4 lists the approximate estimators constructed for distillate composition control. Figure 14 and Figure 15 show the steady state distillate composition error for changes in feed composition for different approximate estimators.

To construct approximate estimators for dual composition control, tray temperatures and steam flow rates were expressed as polynomial functions of reflux flow rate using a least square criterion.

Table 5 lists the approximate estimators constructed for dual composition control. Figure 14, Figure 15, Figure 16 and Figure 17 show steady state composition errors for changes in feed composition for the approximate

Figure 14. Steady State Distillate Composition error for AE1 Estimator and Brosilow's Estimator for Changes in Feed Composition (Dual Composition Control)

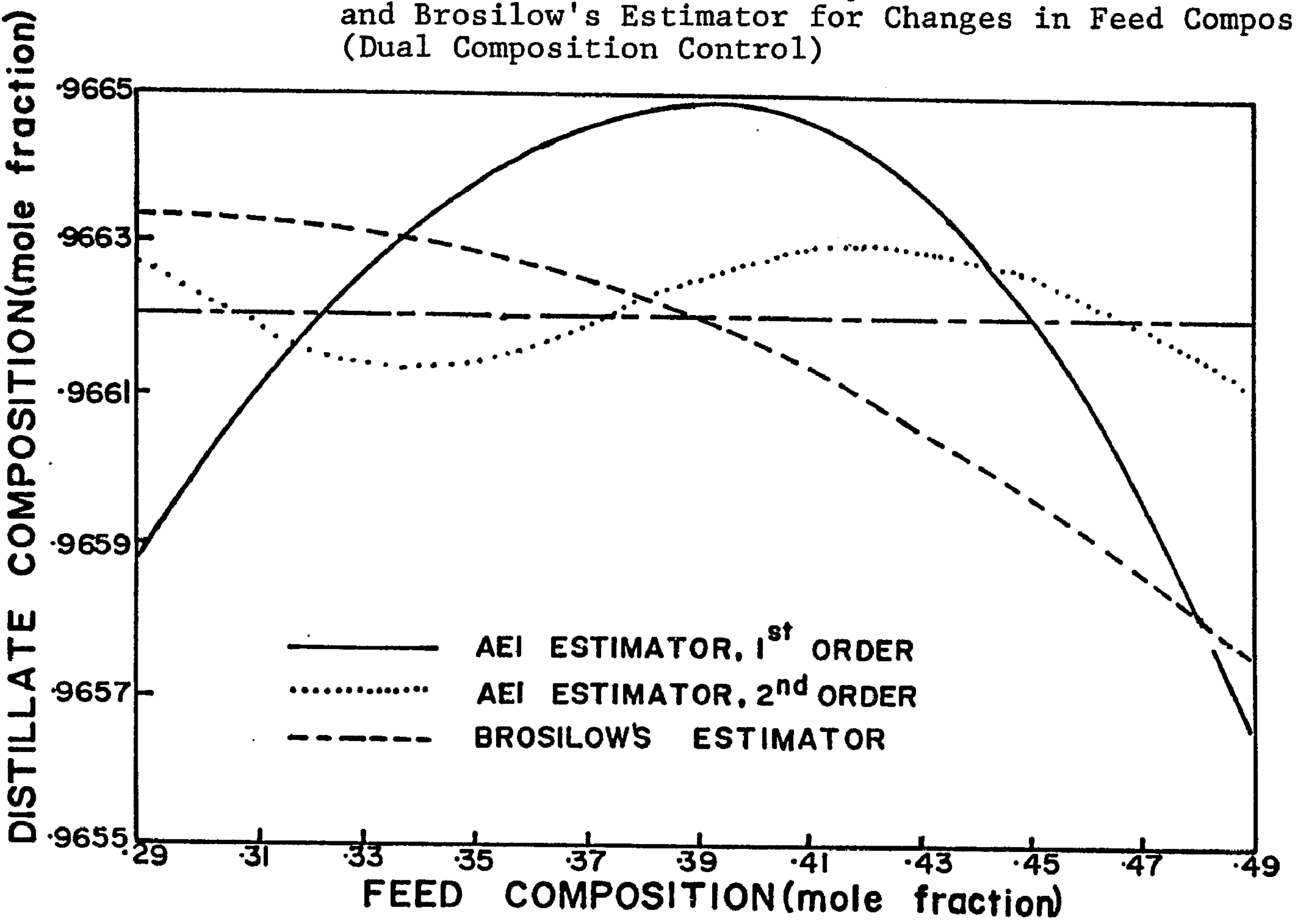
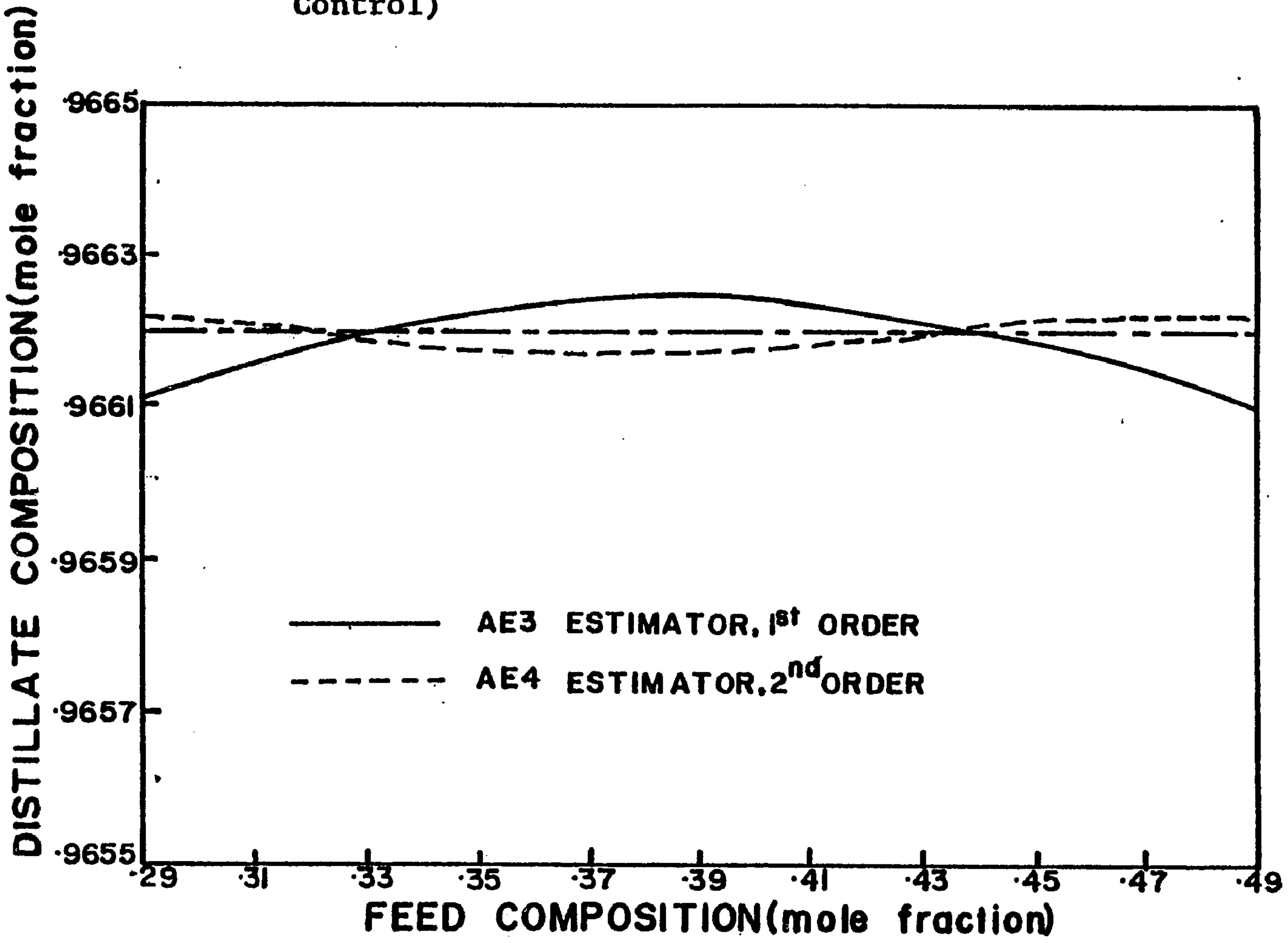


Figure 15. Steady State Distillate Composition Error for AE 3 and AE4 Estimators for Changes in Feed Composition (Dual Composition Control)



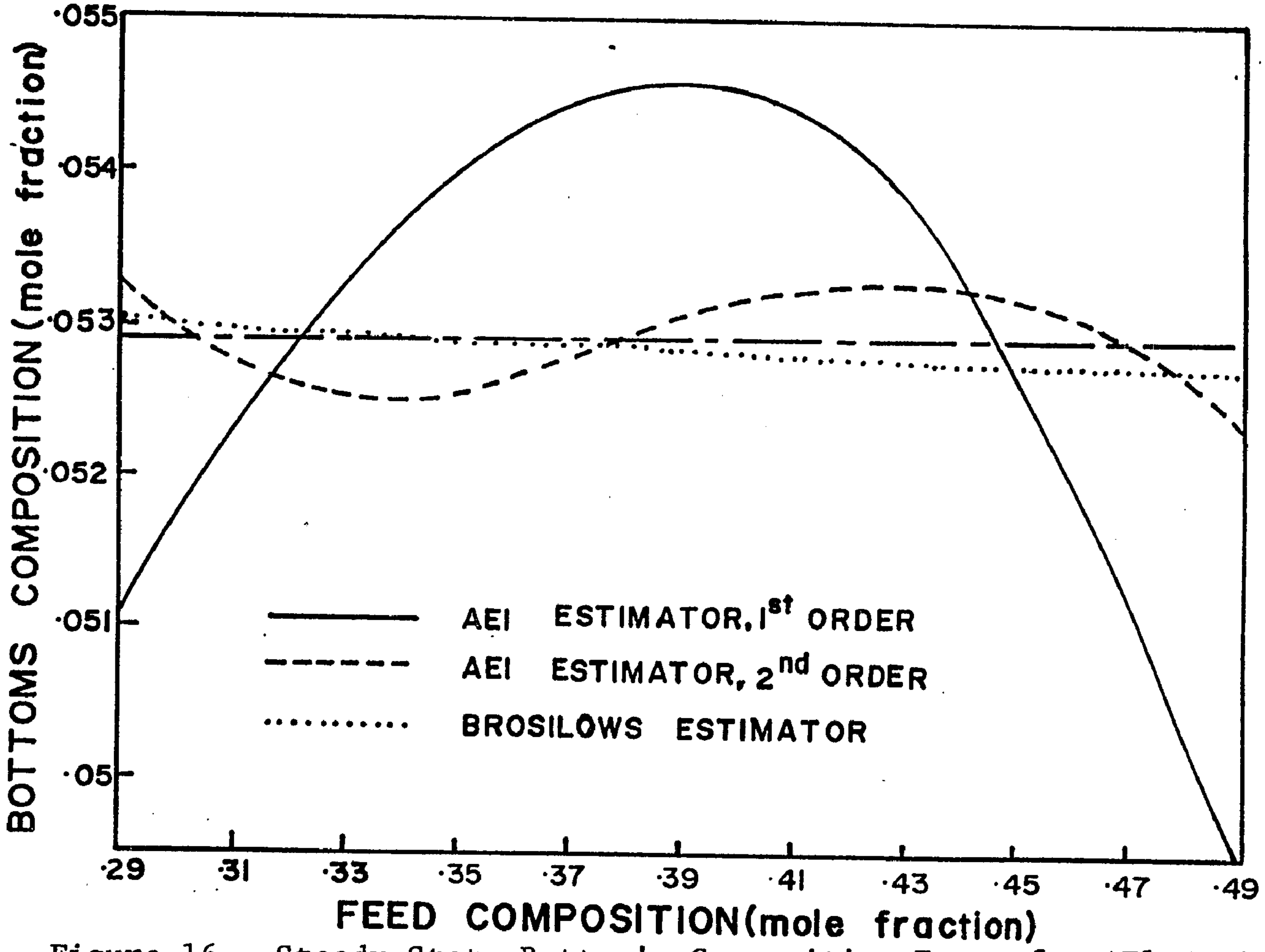


Figure 16. Steady State Bottom's Composition Error for AE1 Estimator and Brosilow's Estimator for Changed in Feed Composition (Dual Composition Control)

Figure 17. Steady State Bottom's Composition Error for AE3 and AE4 Estimators for Changes in Feed Composition (Dual Composition Control)

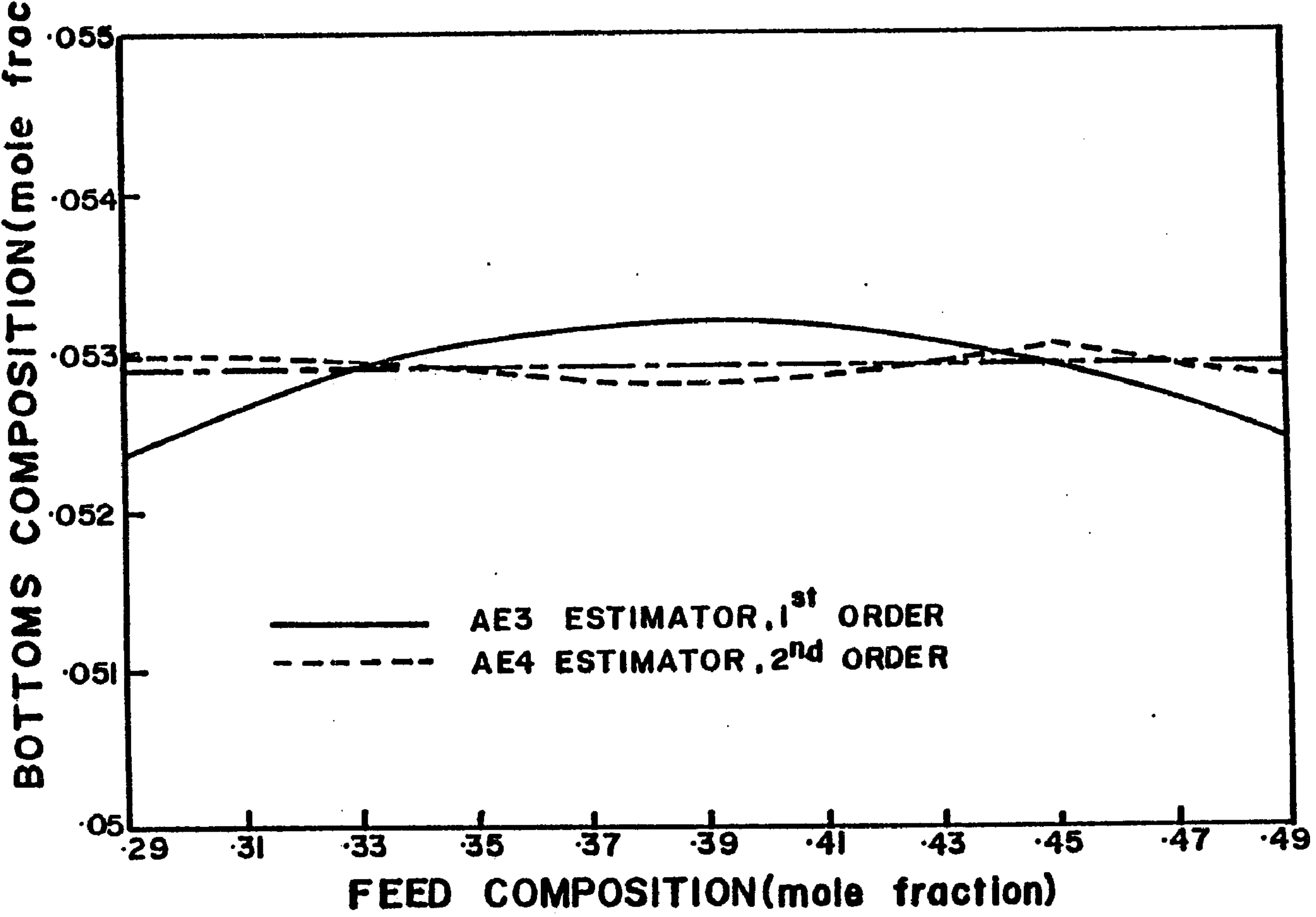


Table 4. Approximate Estimators for Distillate Composition Control

Description	Definition of ϕ*
AE1, 1st order	$\phi 1 = 55.74 + .45\ R - T_{14}$
AE1, 2nd order	$\phi 1 = 58,06 - .337\ R - .0013\ R^2 - T_{14}$
AE2, 1st order	$\phi 2 = -123.75 + 2.22\ T_{14} - R$
AE2, 2nd order	$\phi 2 = -205.80 + 4.43\ T_{14} - .01489\ (T_{14})^2 - R$
AE3, 1st order	$\phi 3 = (-6.27 + .568\ T_4) - (-376.45 + 5.83\ T_{17})$
AE3, 2nd order	$\phi 3 = \{-82.085 + 2.38\ T_4 - .01088\ (T_4)^2\}$
	$\{- 2339.96 - 70.05\ T_{17} + .5299\ (T_{17})^2\}$
AE4, three temperatures	$\phi 4 = T_6 - 190.00 - .009\ T_{10} - 3.68\ T_{15}$

*R - Reflux flow rate gmoles/min.

*T_i - Temperature of i^{th} tray, ^{o}C.

Table 5. Approximate Estimators for Dual Composition Control

Description	Definition of ϕ*
AE1, 1st order	$\phi 1 = 95.84 - .379\ R - T_5$
AE1, 2nd order	$\phi 1 = 81.61 + .349\ R - .0092\ R^2 - T_5$
AE2, 1st order	$\phi 2 = 251.87 - 2.626\ T_5 - R$
AE2, 2nd order	$\phi 2 = -864.69 + 25.01\ T_5 - .157\ (T_5)^2 - R$
AE3, 1st order	$\phi 2 = (272.97 - 2.844\ T_4) - (1477.46 - 20.107\ T_{17})$
AE3, 2nd order	$\phi 3 = \{-1053.016 + 29.48\ T_4 - .1969\ (T_4)^2\}$
	$-\{-70219.33 + 1985.24\ T_{17} - 14.022\ (T_{17})^2\}$
AE4, three temperatures	$\phi 4 = T_8 + 147.78 - .1935\ T_{10} - 2.8611\ T_{14}$

*R - Reflux flow rate, gmoles/min.

*T_i - Temperature of i^{th} tray, ^{o}C.

estimators described in Table 4.

All the approximate estimators designed use optimum tray temperature measurements.

The steady state composition errors for approximate estimators are very small for feed composition changes. It was found that the steady state composition error for AE2 estimators are almost identical to that for AE1 estimator of the same order. The higher the order of the approximate estimators, the smaller the steady state composition error for feed composition changes.

6.5. Steady State Composition Error for Nonlinear Rigorous Estimators

The first step in selecting optimum tray temperatures for rigorous estimators is to investigate the sensitivity of RE1 estimators to measurement errors.

Figure 18 represents sensitivity analysis for RE1 estimator to estimate distillate composition. 1% measurement error in process flow rates and .1°C tray temperature measurement error was assumed.

Figure 19 represents sensitivity analysis of RE1 estimator to estimate bottom's product composition for 1% measurement errors in process flow rates and .1°C tray temperature measurement error.

Tray 14 temperature was selected as an optimum tray temperature for RE1 estimator to estimate distillate composition. Temperatures of trays 12, 14, 16 and 18 were

Figure 18. Sensitivity Analysis for Binary Methanol/Water Column for RE1 Estimator (Distillate Composition Control)

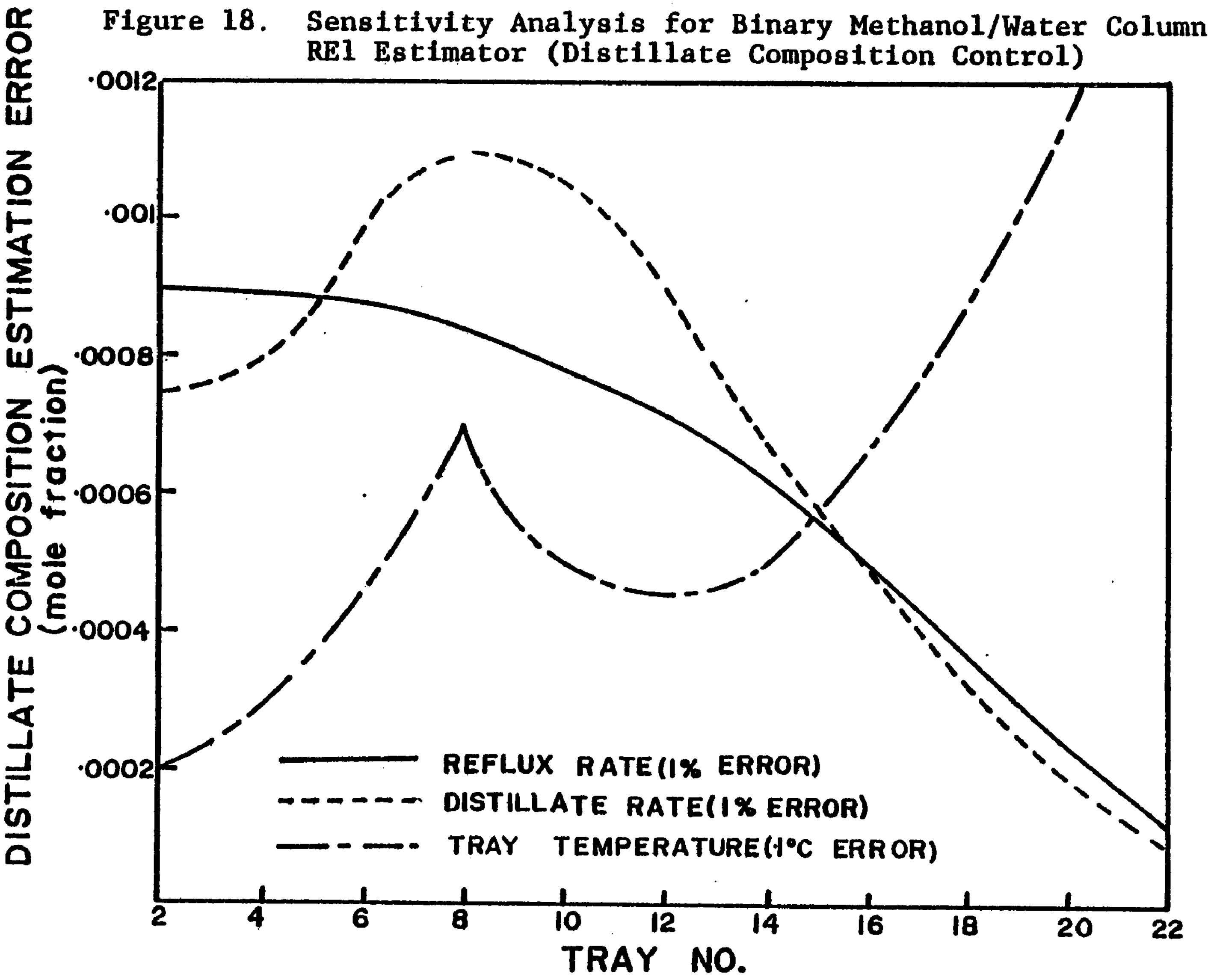
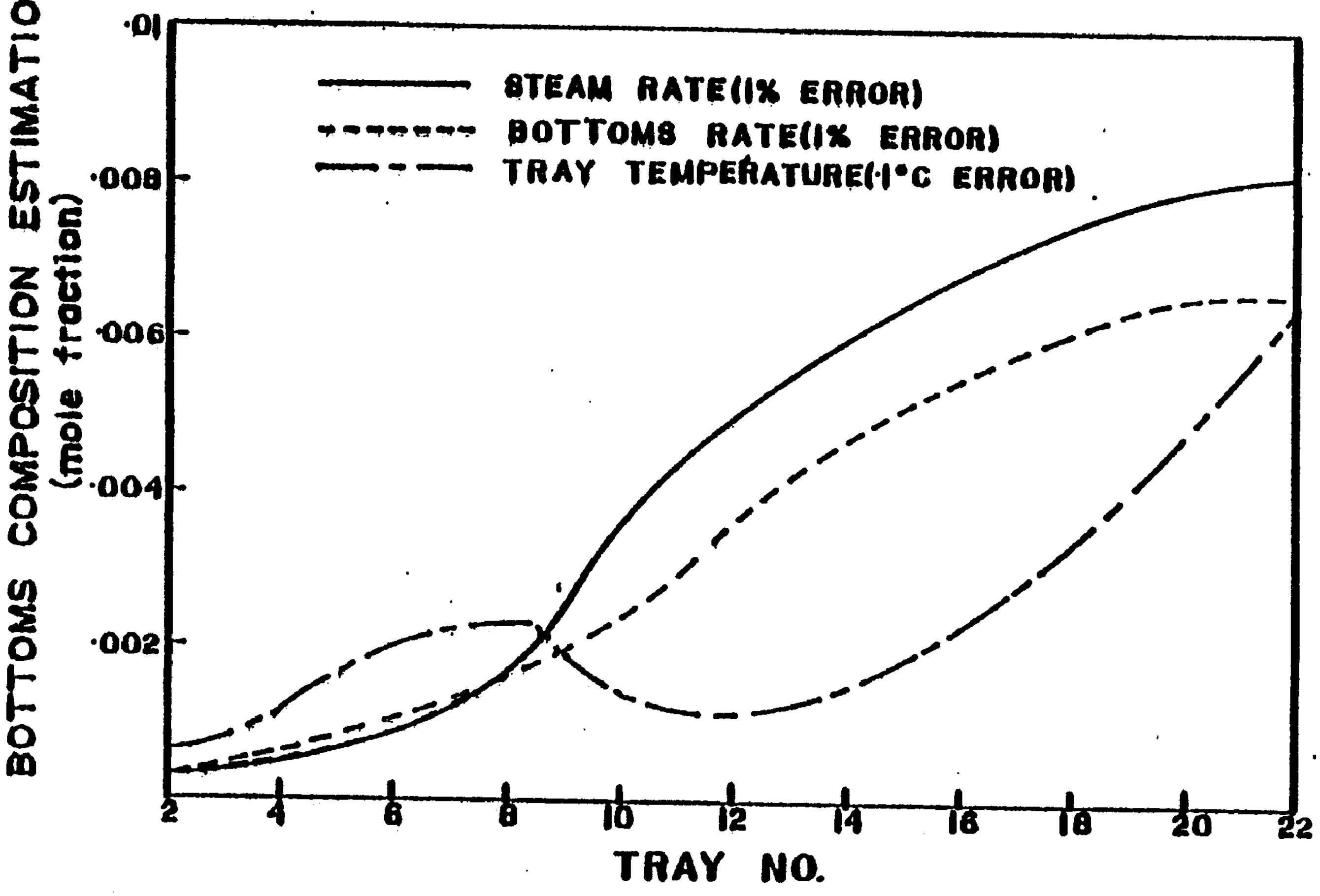


Figure 19. Sensitivity Analysis for Binary Methanol/Water Column for REI Estimator (Bottom's Product Composition Control)



selected as optimum tray temperatures for RE2 and RE3 estimators to estimate the distillate composition.

Tray 4 temperature was selected as an optimum tray temperature for RE1 estimator to estimate bottom's product composition. Temperatures of trays 2,3,4 and 5 were optimum tray temperatues selected for RE2 and RE3 estimators to estimate the bottom's product composition.

Rigorous estimators would not give any steady state product composition errors for changes in feed stream parameters and/or composition set point changes assuming no modelling or measurement errors.

Figure 20 and Figure 21 show the sensitivity of RE1 estimator to changes in column parameters. The column parameters considered were tray efficiencies, tray heat losses and tray pressure drops.

The rigorous estimators are very sensitive to changes in tray efficiencies but relatively insensitive to changes in tray heat losses and tray pressure drops.

6.6. Discussion of Results

For the binary methanol/water column, the steady state product composition errors associated with estimator based control schemes are negligibly small compared with conventional control strategy of controlling a tray temperature for changes in feed composition.

Large steady state bottom's product composition errors were observed in case of Brosilow's linear esti-

Figure 20. Sensitivity of RE1 Estimator to Modelling Errors for Binary Methanol/Water Column (Bottom's Product Composition Control)

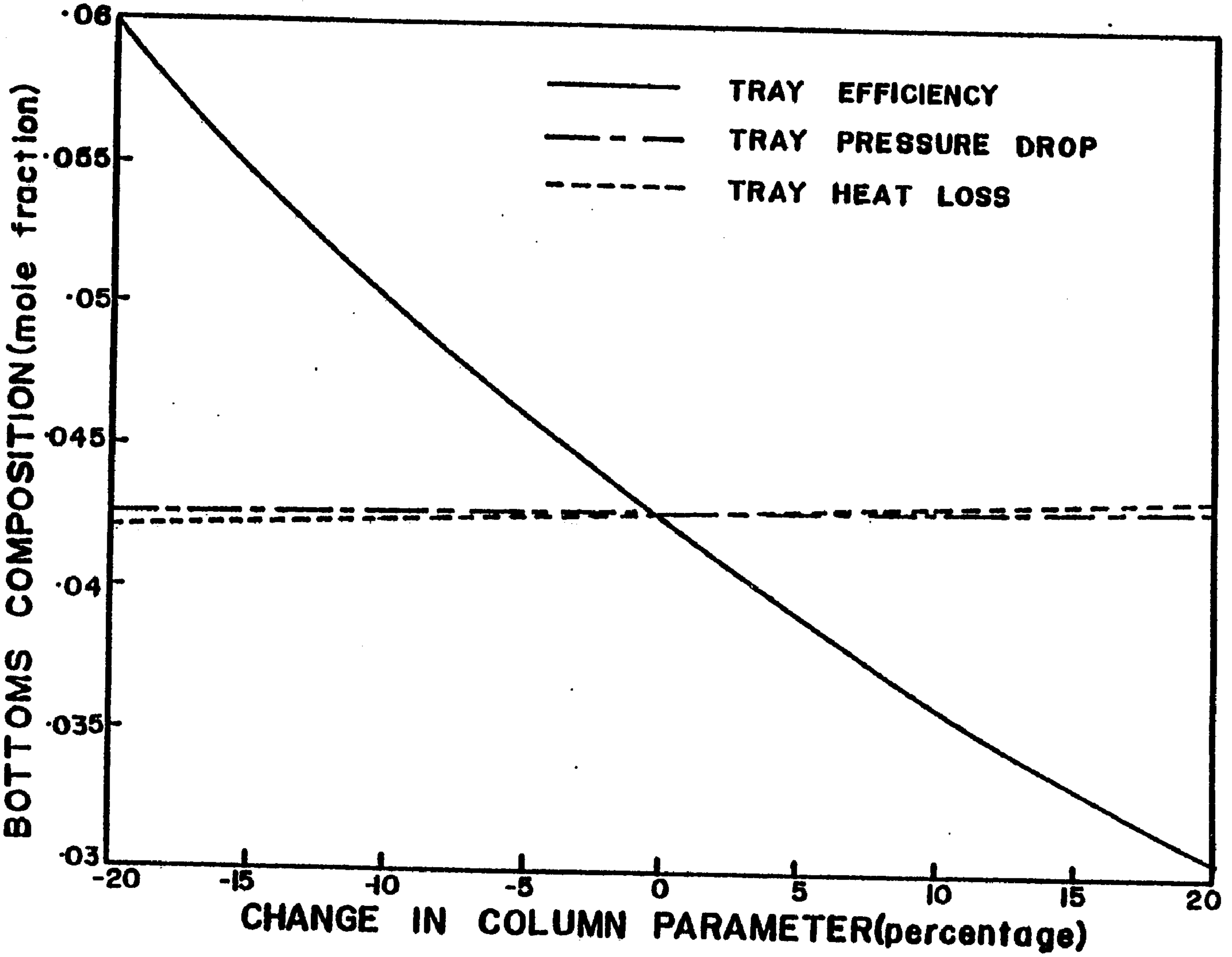
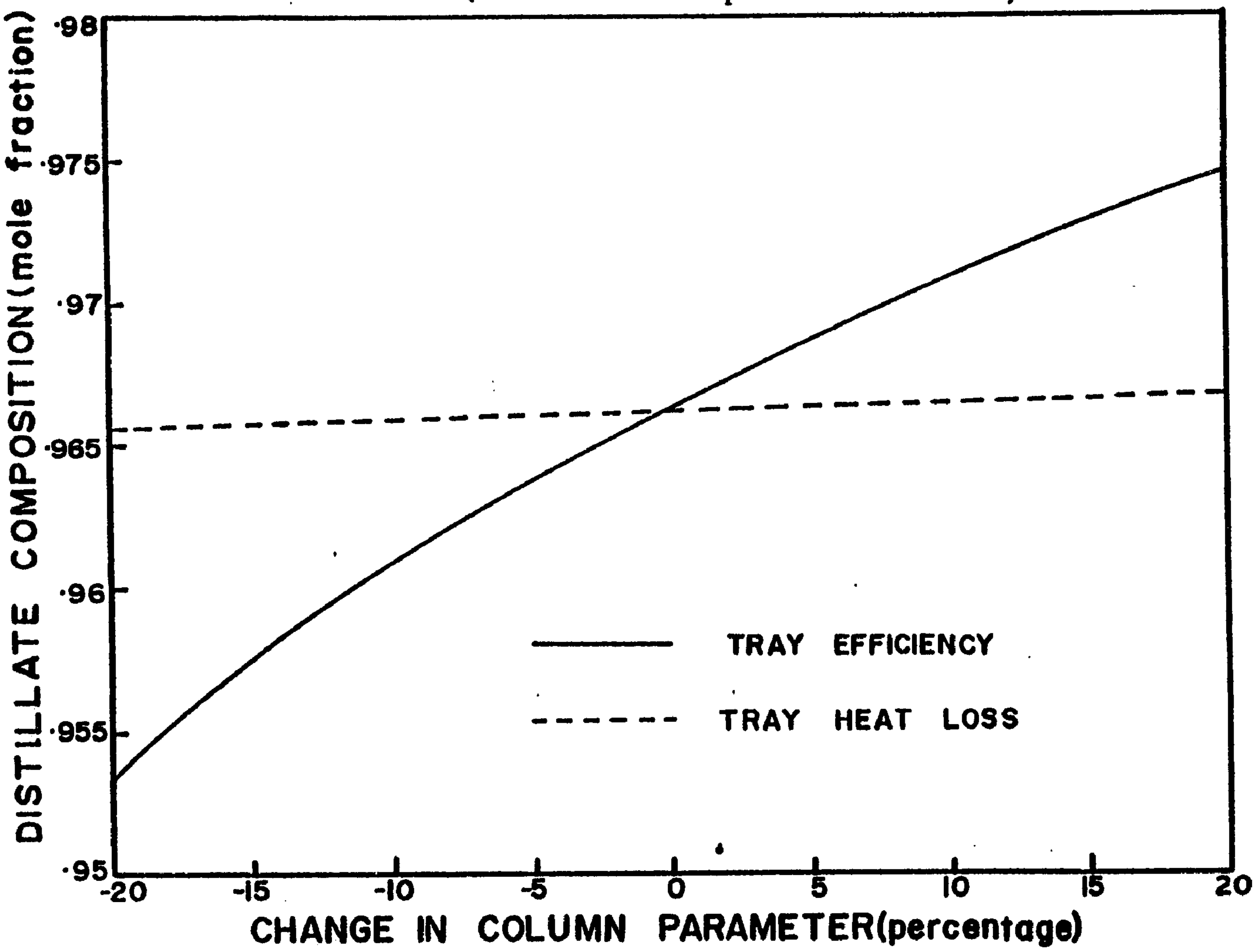


Figure 21. Sensitivity of RE1 Estimator to Modelling Errors for Binary Methanol/Water Column (Distillate Composition Control)



mator for changes in bottom's composition set points. The rigorous estimators are superior to Brosilow's linear estimator in this respect.

7. DYNAMIC SIMULATION

The techniques using composition estimation were tested on the dynamic model of the column. The objective of the study was to compare the effectiveness of various estimators and to compare conventional feedback control schemes with inferential control techniques using estimators.

The column was subject to feed composition step disturbance (-5 percent) when the control objective was distillate composition control or dual composition control. The column response was also studied for setpoint changes in bottom's product composition.

7.1 Dynamic Model

The model involves tray to tray energy and material balances. Additional assumptions besides those made in static model were i) negligible vapor holdup, ii) dead time in reflux piping and reboiler. The differential equations describing the column were integrated using simple Euler's integration algorithm. Details of the computational procedure are given in a thesis by Tyreus (10).

To evaluate the accuracy of the dynamic model described, simulated transient responses and dynamic responses of the experimental column were compared for a i) step disturbance in reflux flow rate, ii) step disturbance in steam flow rate.

Figure 22 shows the transient tray temperature responses for a step change in reflux flow from .495 gpm to .55 gpm. Figure 23 shows the transient tray temperature responses for a step change in steam flow rate from .358 kg/min to .382 kg/min. The agreement between the simulated and experimental dynamic responses is good.

7.2 Distillate Composition Control

The control objective is to maintain the distillate composition on target value in face of a step change in feed composition (-5 percent) by manipulating reflux flow rate. Reboiler heat load is constant.

The conventional feedback control schemes explored were i) direct distillate composition control assuming no measurement lags, ii) controlling column overhead vapor composition, iii) controlling a tray temperature in the rectifying section.

The inferential composition control was achieved by controlling the value of ϕ (described in Table 2) for approximate estimators.

In case of Brosilow's linear estimator and rigorous estimators, the estimated distillate composition was controlled.

The transfer functions of controlled variables with respect to reflux flow rate were obtained by pulse testing the dynamic model and subsequent fourier analysis of the transients.

Figure 22. Transient Tray Temperature Responses for a Step Change in Reflux Flow Rate

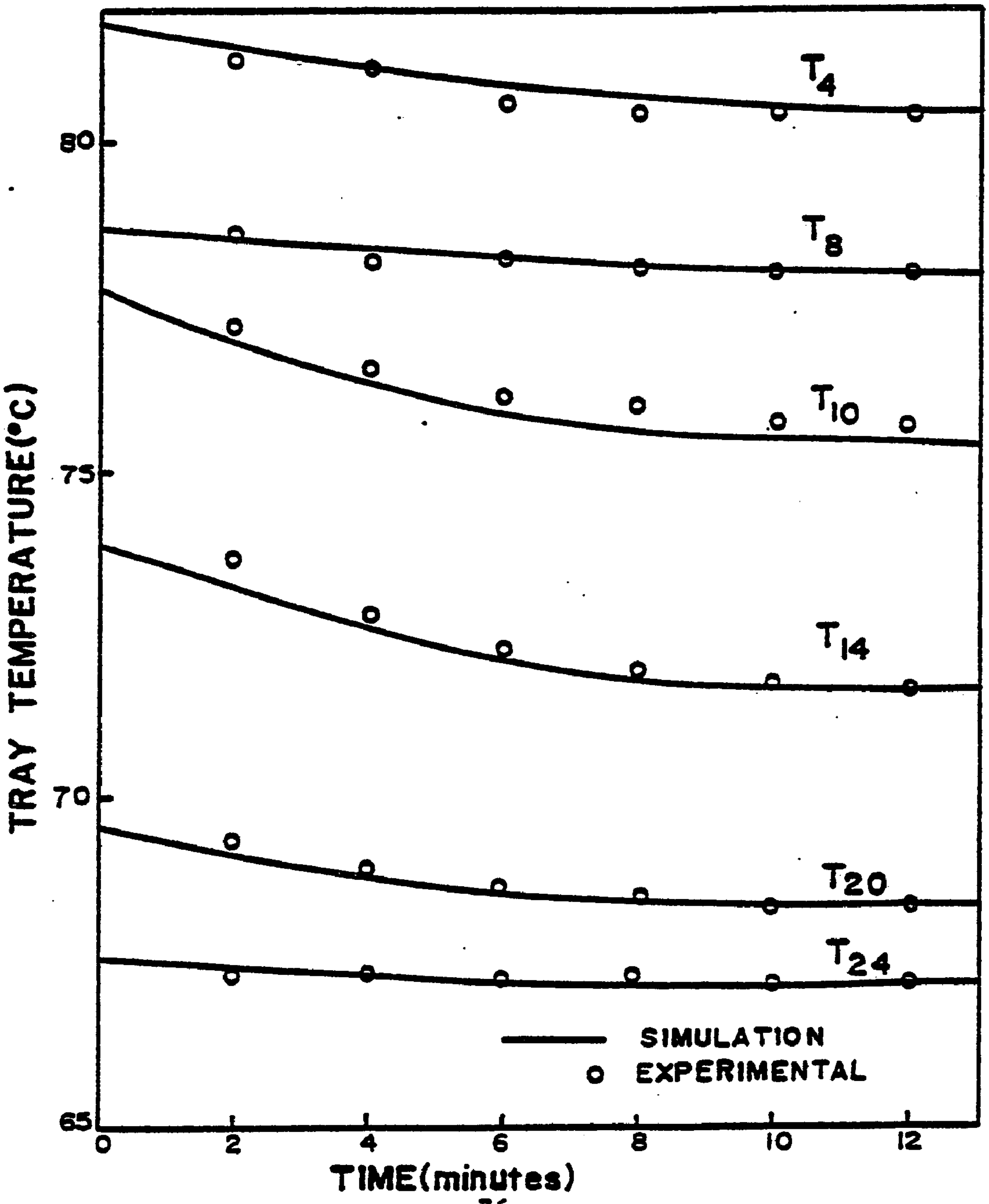
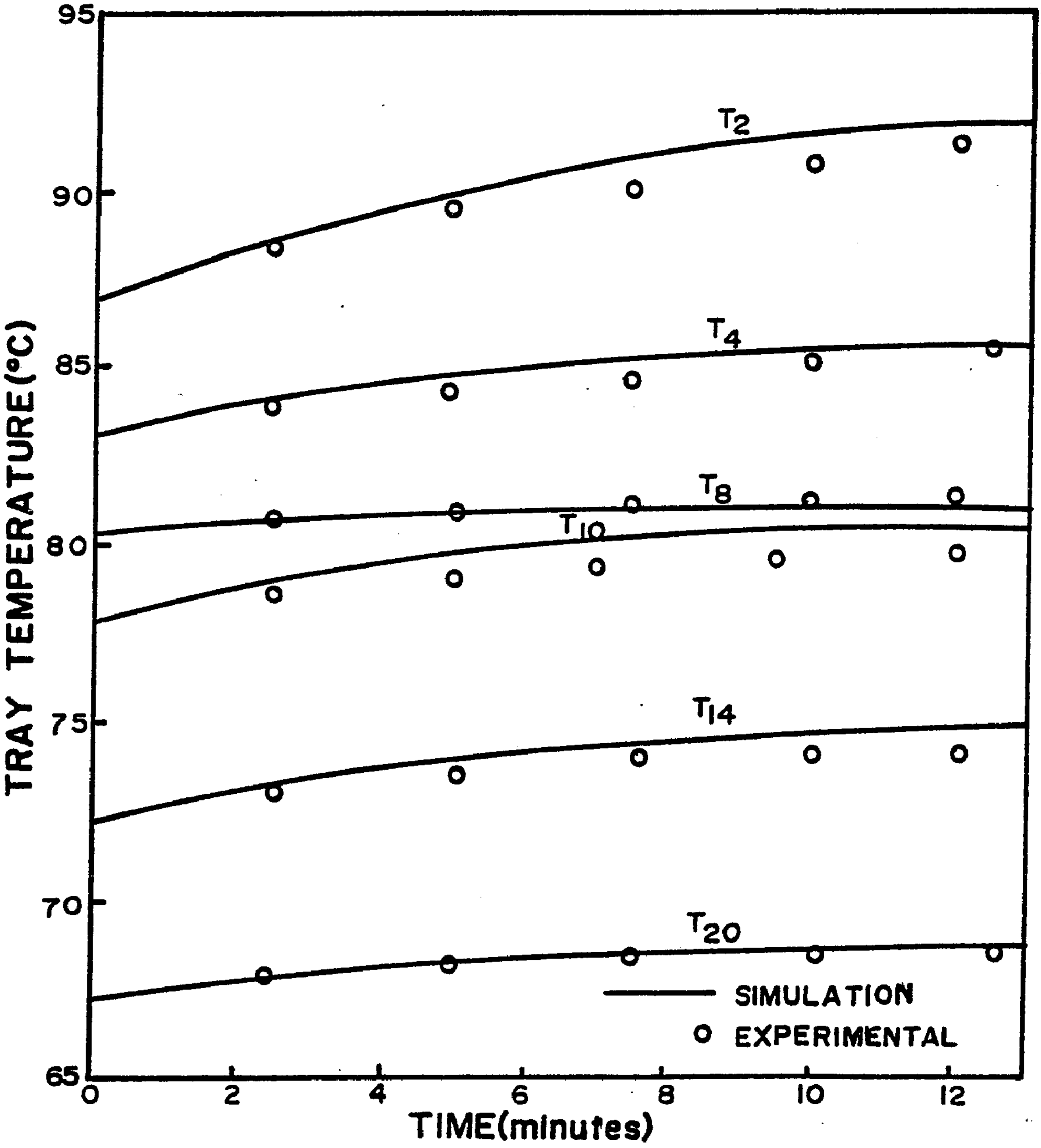


Figure 23. Transient Tray Temperature Responses for a Step Change in Steam Flow Rate



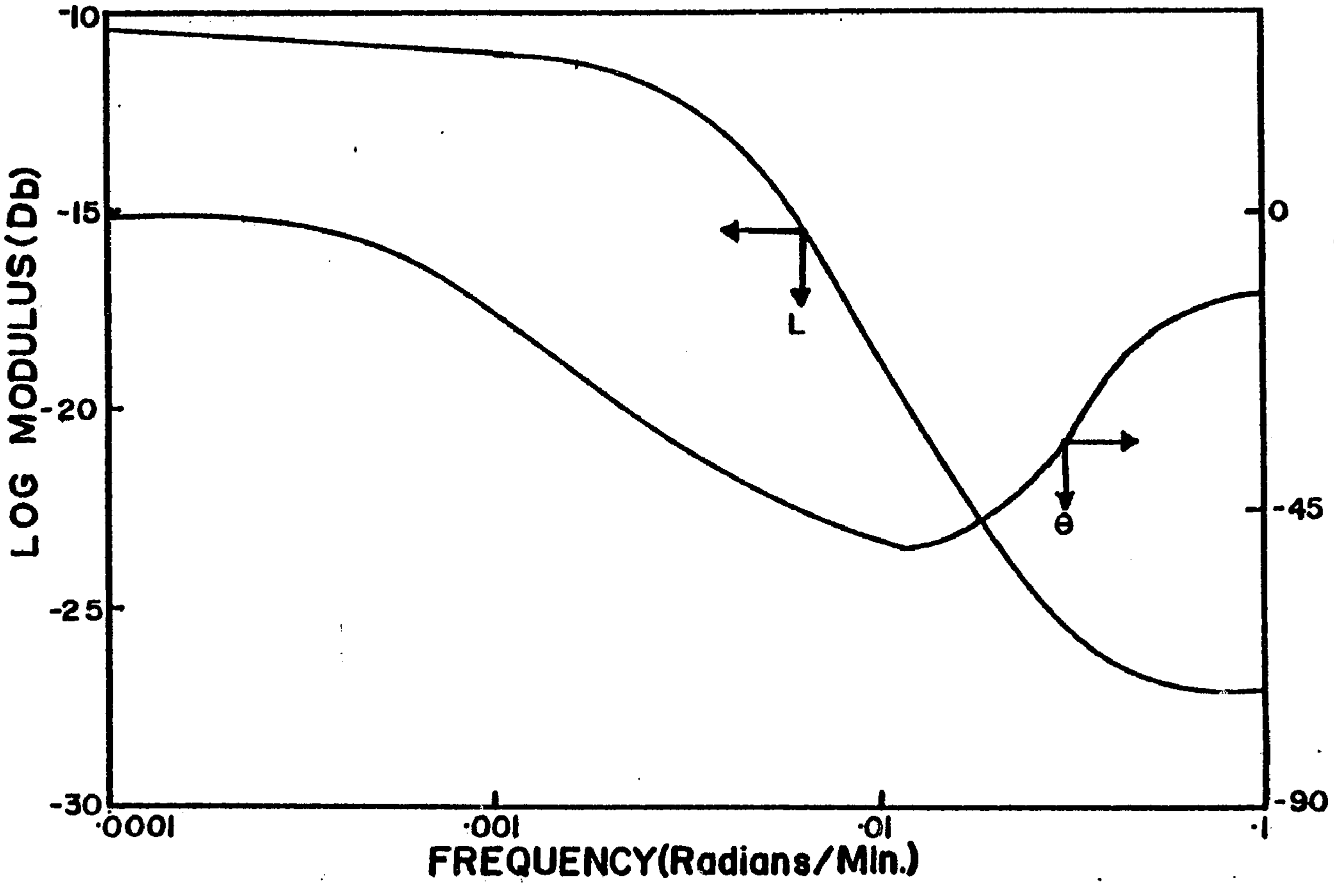
In case of rigorous estimators, the transfer function for estimated distillate composition with respect to reflux flow rate could not be defined in terms of first order or second order lag with dead time. Typical Bode plots for the transfer function for RE1 estimator are shown in Figure 24. A first order lead time appears to be present. This means more stable closed loop control system.

The PI controller settings for conventional control schemes were calculated using process transfer functions. The controller reset time was determined based on Ziegler-Nichol's criterion. The controller gain was calculated so that the damping coefficient was 0.5 in frequency domain.

For approximate estimators and Brosilow's linear estimator, the controller reset time was calculated in similar fashion. In case of AE1 and AE2 estimators, the control system was found to be closed loop stable for all values of controller gain. In case of AE3 estimator, AE4 estimator and Brosilow's linear estimator the response of the simulated nonlinear column was overdamped if controller gain was selected such that damping coefficient was 0.5. Hence, the controller gains for these estimator based control schemes were determined by further tuning of the controller using simulated response of the column.

The PI controllers for control schemes based on rigorous estimators were tuned by trial and error using

Figure 24. Bode Plots for Transfer Function for RE1 Estimator (Estimated Distillate Composition with Respect to Reflux Flow Rate)



simulated response of the column.

Table 6 shows the transfer functions and controller settings used for the control schemes described.

Figure 25 shows the open loop response of the column subject to a feed composition disturbance of -5 percent. Figure 26 shows the responses of the column for conventional composition control strategies. Figure 27 and Figure 28 shows the responses of the column for estimator based control schemes.

In general, the control achieved by using estimator based inferential control schemes is superior compared with conventional control schemes. The control system is more stable and steady state composition errors are negligible. However, poor control is achieved when RE2 estimator based control scheme is implemented due to dynamics of the column. The control systems based on RE1 and RE3 estimators are more stable compared to control systems based on other estimators.

7.3. Bottom's Product Composition Control

The bottom's product composition control was achieved by manipulating steam flow rate (reflux flow rate is constant).

The responses of the column for a step change in bottom's product composition setpoint using control schemes based on i) Tray 4 temperature control, ii) Brosilow's linear estimator, iii) RE1 estimator, iv) RE3 estimator were compared.

Figure 25. Open Loop Response of the Column for a Step Change in Feed Composition

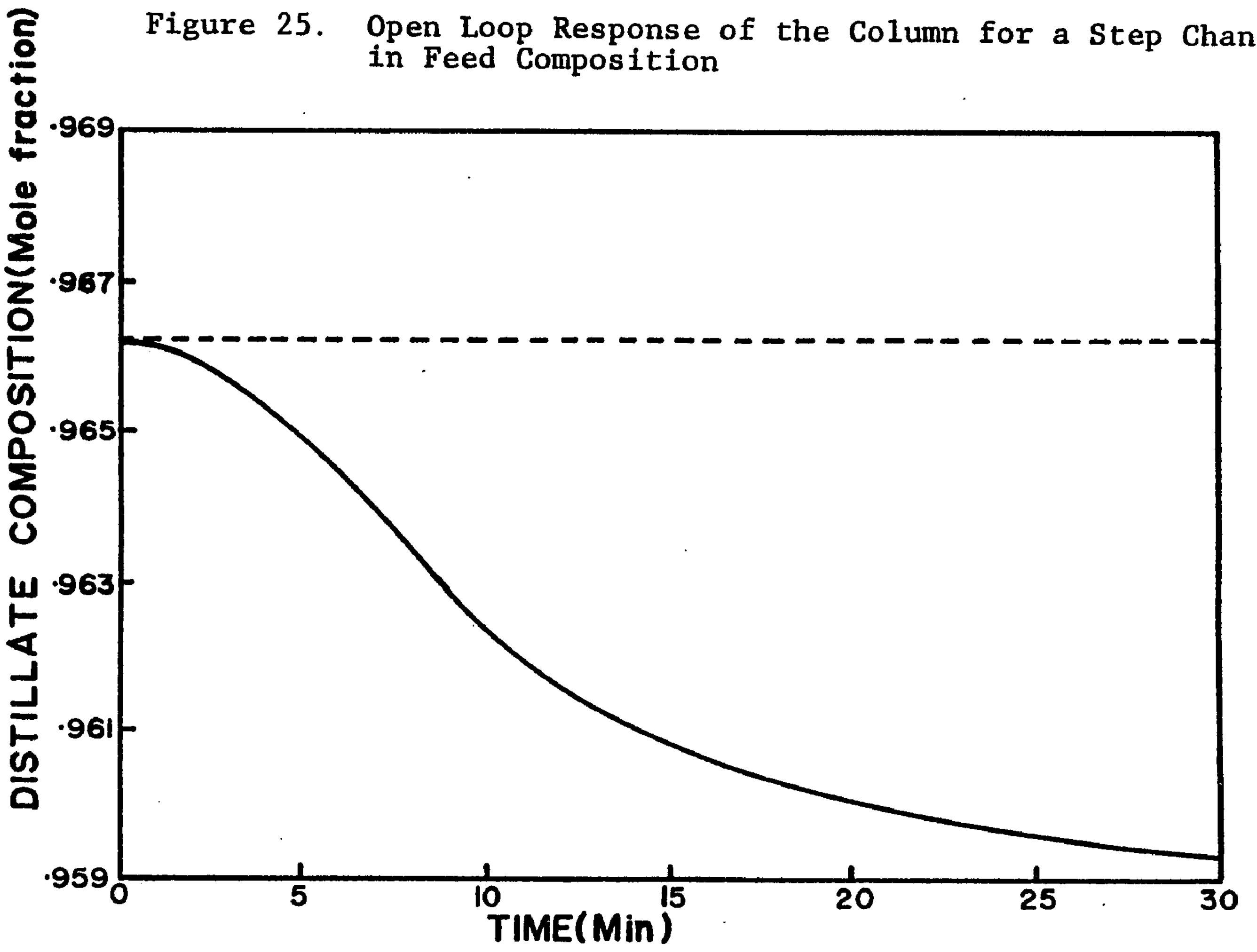


Figure 26. Response of the Column for Conventional Control Schemes for a Step Change in Feed Composition (Distillate Composition Control)

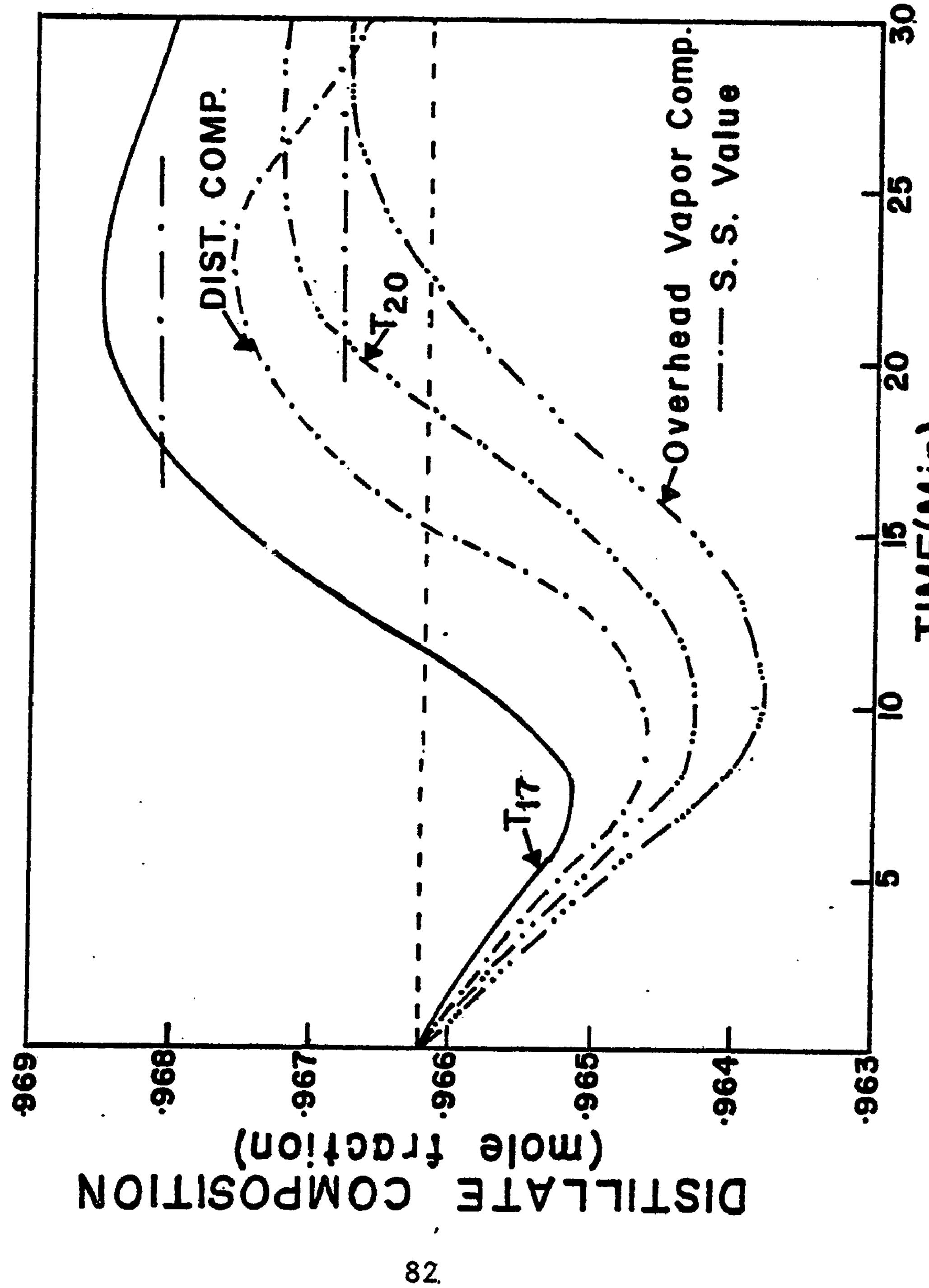


Figure 27. Dynamic Responses of the Column for Approximate Estimator Based Control Schemes (Distillate Composition Control) for a Step Change in Feed Composition

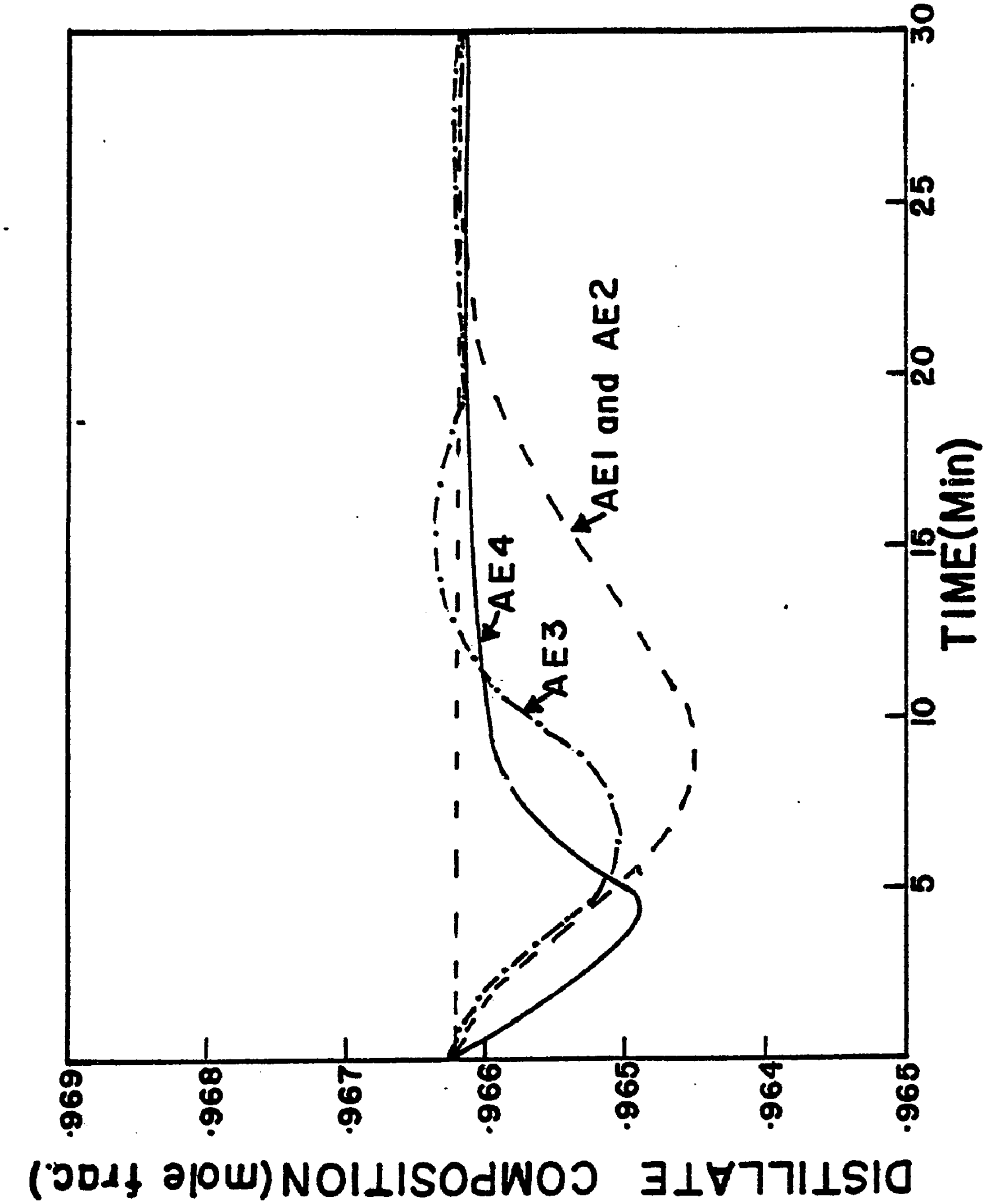


Figure 28. Dynamic Responses of the Column for Brosilow's Linear Estimator and Rigorous Estimators Based Control Schemes (Distillate Composition Control) for a Step Change in Feed Composition

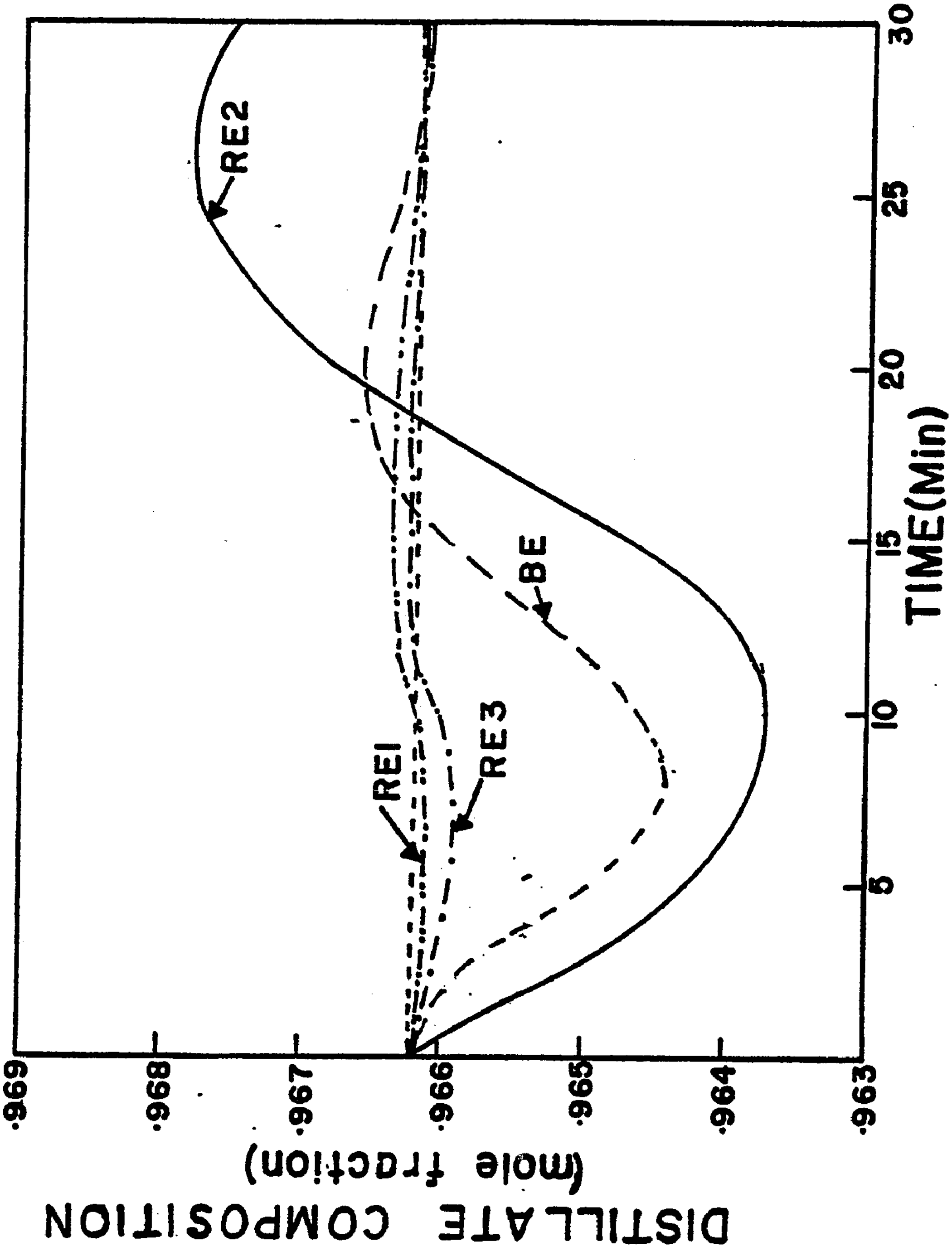


Table 6. Transfer Functions with Respect to Reflux Flow Rate and Controller Settings for Various Distillate Composition Control Schemes

Control Scheme	Control Variable	Transfer Function	Controller Settings	
			Gain**	Reset Time (min.)
Direct Distillate Composition Control	Distillate Composition	$\frac{.0052e^{-.2S}}{(7S+1)(2.3S+1)}$ $\frac{\text{mole fraction}}{\text{g-mole/min}}$	96.	2.91
Control of Overhead Vapor Composition	Overhead Vapor Composition	$\frac{.0052e^{-.7S}}{(7S+1)}$ $\frac{\text{mole fraction}}{\text{g-mole/min}}$	103.56	1.4
Control of Tray 17 Temperature	Tray 17 Temperature	$\frac{.567e^{-.7S}}{(6S+1)}$ ^{o}C/g-mole/min	1.044	1.73
Brosilow's Linear Estimator	Estimated Distillate Composition	$\frac{.0053e^{-.65S}}{(6S+1)}$ $\frac{\text{mole fraction}}{\text{g-mole/min}}$	180.	1.88
*AE1 Estimator 2nd order	$\phi 1$	$(\frac{.715e^{-.83S}}{(5.8S+1)} + 27)\frac{^{o}C}{\text{g-mole/min}}$	1.2	2.0
*AE2 Estimator 2nd order	$\phi 2$	$(\frac{-1.455e^{-.8S}}{(5.6S+1)} - 1)\frac{\text{g-mole/min}}{\text{g-mole/min}}$	.72	1.9
*AE3 Estimator 2nd order	$\phi 3$	$\frac{3e^{-.7S}}{(5.9S+L)}$ $\frac{\text{g-mole/min}}{\text{g-mole/min}}$	.6	1.8
*AE4 Estimator, Three Temperatures	$\phi 4$	$\frac{2.147e^{-.77S}}{(5.8S+1)}$ $\frac{^{o}C}{\text{g-mole/min}}$	6.	1.9
RE1 Estimator	Estimated Distillate Composition		360.	0.5
RE2 Estimator	" "		96.	1.5
RE3 Estimator	" "		180.	0.75

* As defined in Table 3.

** The units are reciprocal of units for the corresponding transfer function.

For the tray 4 temperature control, the tray 4 temperature setpoint change corresponding to the step change in bottom's composition setpoint was calculated using the steady state model of the column.

The process transfer functions and controller settings were obtained by the same procedure as described in the previous section. Table 7 lists the transfer functions and controller settings.

Figure 29 shows the responses of the column for the control schemes described.

Poor control was observed for control scheme based on Brosilow's linear estimator because of large steady state composition error.

7.4. Dual Composition Control

Dual composition control was achieved in face of -5 percent step change in feed composition by manipulating reflux flow rate and steam flow rate simultaneously.

The responses of the column for inferential composition control techniques based on 1) controlling two tray temperatures, 2) Brosilow's linear estimator, 3) approximate estimators, 4) rigorous estimators RE1 and RE3 were compared.

In case of Brosilow's linear estimator and rigorous estimator based control schemes, the estimated distillate composition and estimated bottom's product composition

Figure 29. Dynamic Responses of the Column for Various Composition Control Schemes (Composition Setpoint Change)

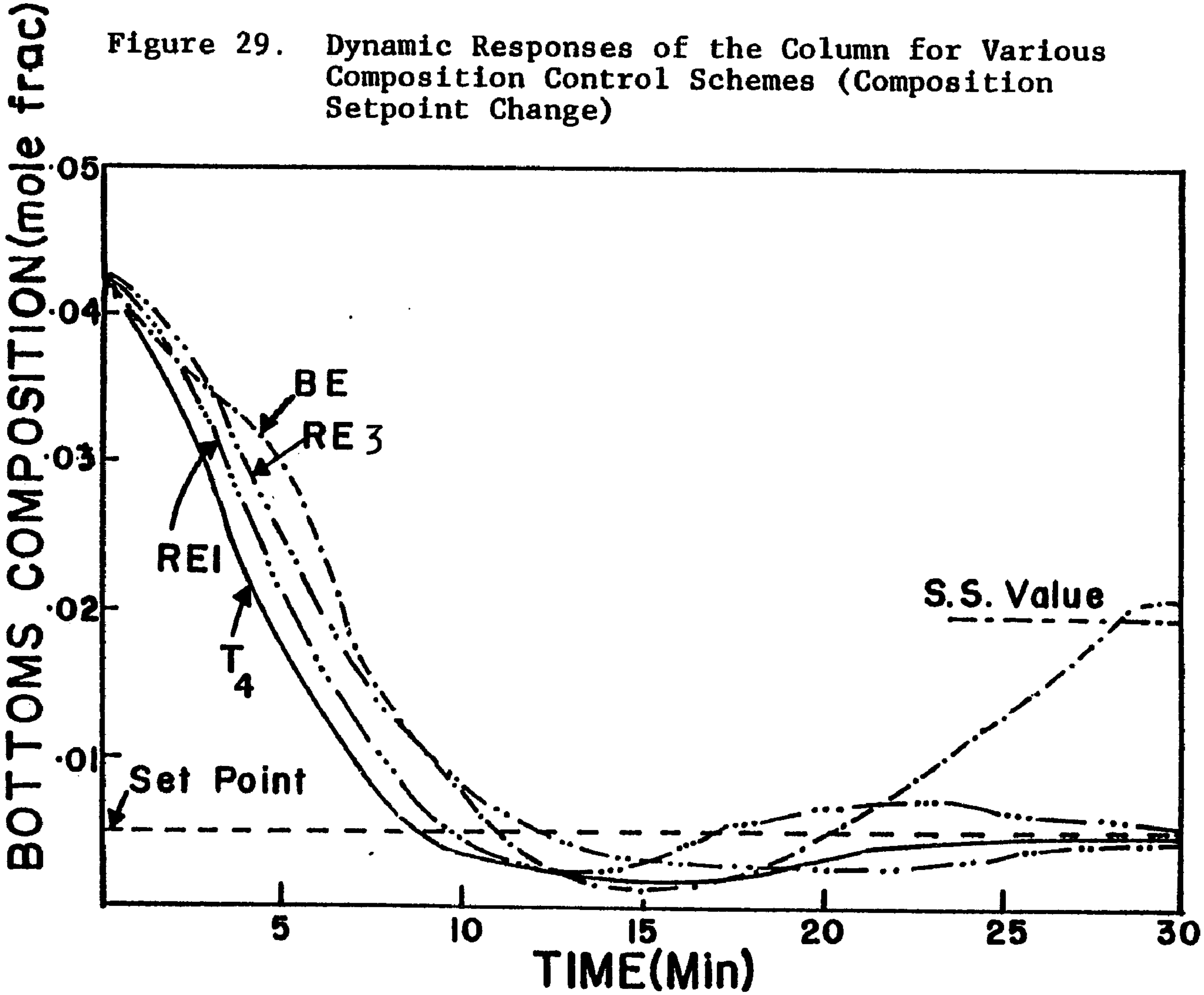


Table 7. Transfer Functions with Respect to Steam Flow Rate and Controller Settings for Various Bottom's Product Composition Control Schemes

Control Scheme	Control Variable	Transfer Function	Controller Settings	
			Gain*	Reset Time (min)
Controlling Tray 4 Temperature	Tray 4 Temperature	$\frac{.457\ e^{-.15}}{(4.8S+1)}\ \frac{{}^{o}C}{\text{g-mole/min}}$	.202	0.5
Brosilow's Linear Estimator	Estimated Distillate Composition	$\frac{.008e^{-.15}}{(4.7S+1)}\ \frac{\text{mole fraction}}{\text{g-mole/min}}$	17.6	0.5
RE1 Estimator	"		50.4	0.5
RE3 Estimator	"		50.4	0.8

*The units are reciprocal of the units for the corresponding transfer function.

were controlled by manipulating reflux flow rate and steam flow rate, respectively.

For approximate estimator based control schemes, the value of ϕ (as defined in Table 4) was controlled by manipulating reflux flow rate while varying steam flow rate as a predetermined function of reflux flow rate.

For approximate estimators, the transfer functions for ϕ with respect to reflux flow rate were obtained by pulse testing (steam flow rate also pulsed as a predetermined function of reflux flow rate simultaneously) and subsequent fourier analysis. The PI controller reset time was determined using Ziegler-Nichol's criterion. The controller gain was selected such that damping coefficient was 0.5. However, the response of the column was overdamped. The controller settings were further tuned by trial and error using simulated response of the column.

For other control schemes, the controller settings obtained by independent tuning of the top and bottom control loops were used (using the procedure described in previous sections). Although the individual control loops are closed loop stable, the overall closed loop control system may not be necessarily stable due to interaction between control loops. The stability of the closed loop control system depends on the characteristic equation.

$$1 + G = 0$$

where

$$G = B_1P_{11}+B_2P_{22}+B_1B_2(P_{11}P_{22}-P_{12}P_{21})$$

where

$B_1(S)$	Transfer function for the top loop controller
$B_2(S)$	Transfer function for the bottom loop controller

$P_{11}(S)$, $P_{21}(S)$ are transfer functions for the top loop and bottom loop control variables with respect to reflux flow rate.

P_{21} and P_{22} are transfer functions for top loop and bottom loop control variables with respect to steam flow rate.

Table 8 and Table 9 list the process transfer functions and controller settings for dual composition control schemes.

The stability of the closed loop control system for control schemes i) controlling two tray temperatures, and ii) based on Brosilow's linear estimator was verified by making Nyquist plots for G as shown in Figure 30 and Figure 31.

Figure 32 to Figure 35 show the simulated responses of the column for various control schemes described. The disturbance was -5 percent step change in feed composition.

It can be concluded that dual composition control can be achieved by using estimator based control schemes.

Figure 30. Nyquist Plot of G for Control Scheme Involving Control of Two Tray Temperatures

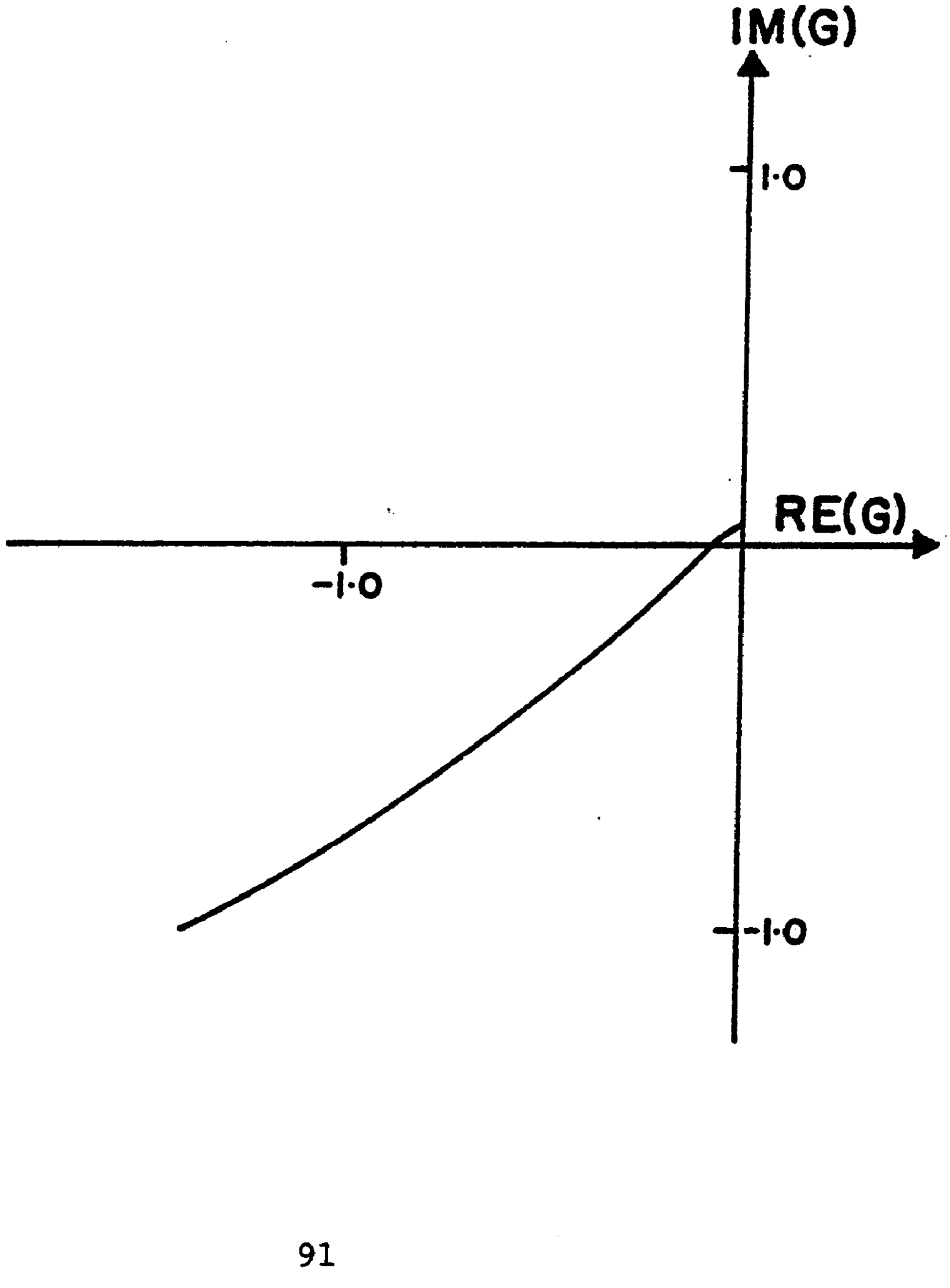
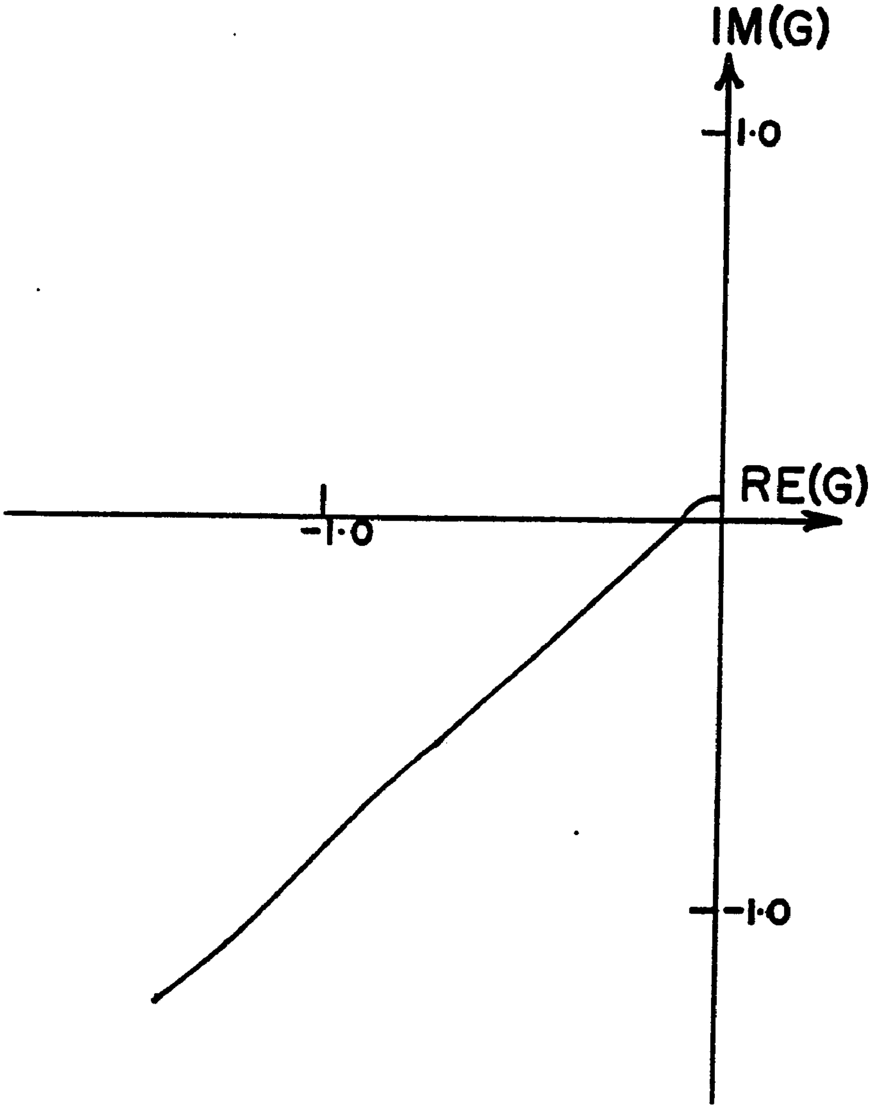


Figure 31. Nyquist Plot of G for Control Scheme Based on Brosilow's Linear Estimator (Dual Composition Control)



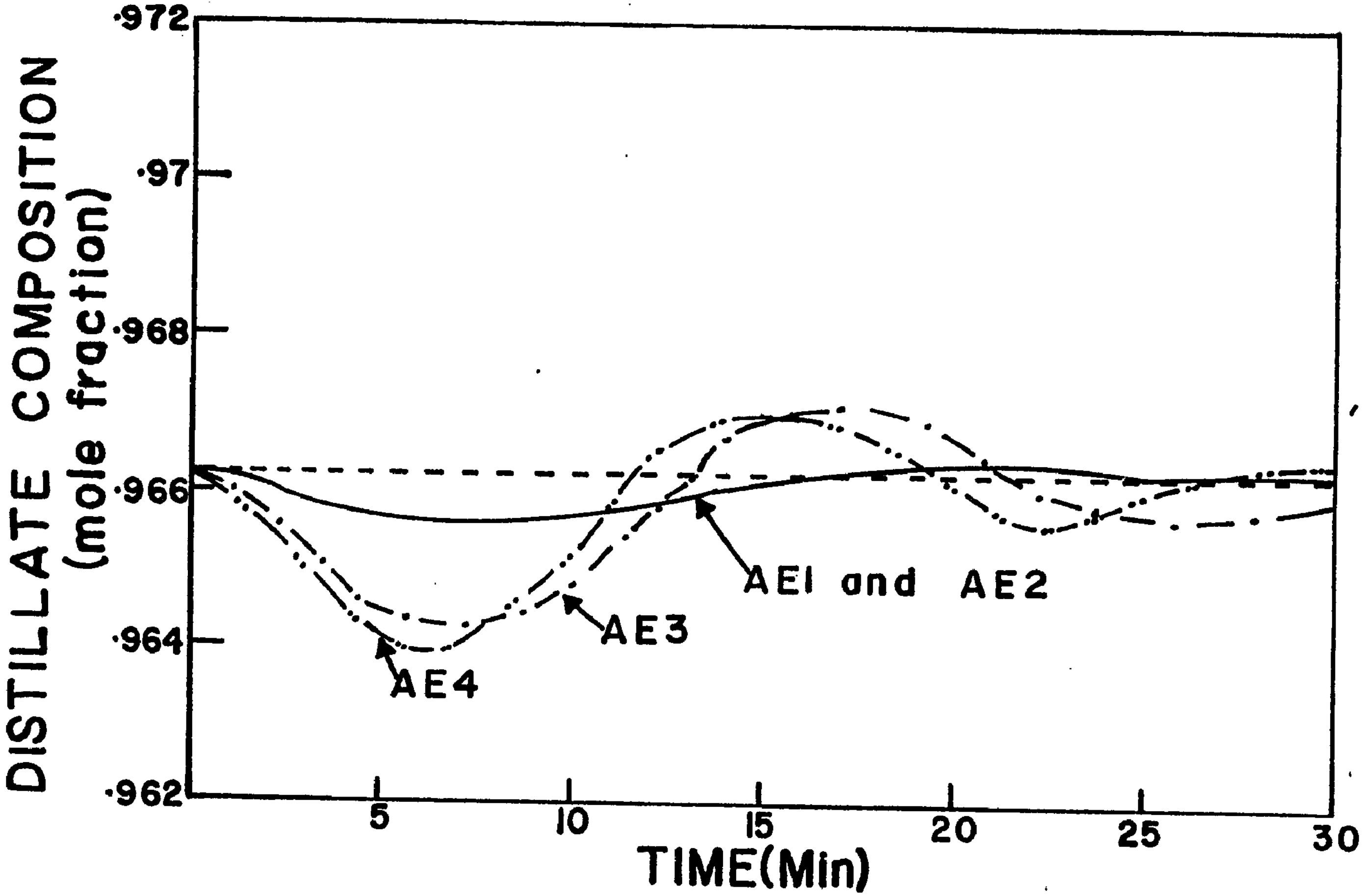


Figure 32. Distillate Composition Responses for Approximate Estimator Based Dual Composition Control Schemes for a Step Change in Feed Composition

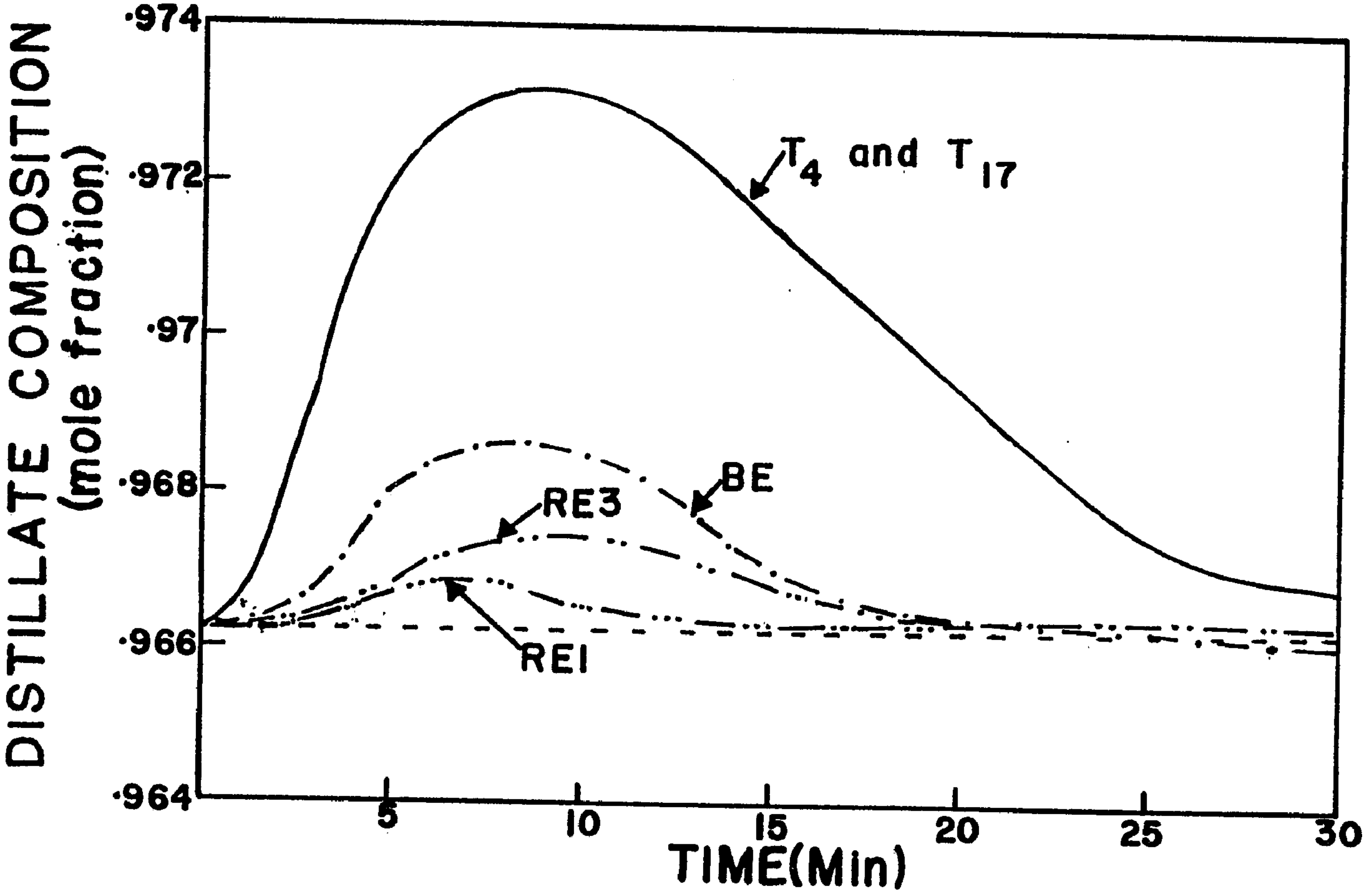


Figure 33. Distillate Composition Responses for Dual Composition Control Schemes for a Step Change in Feed Composition

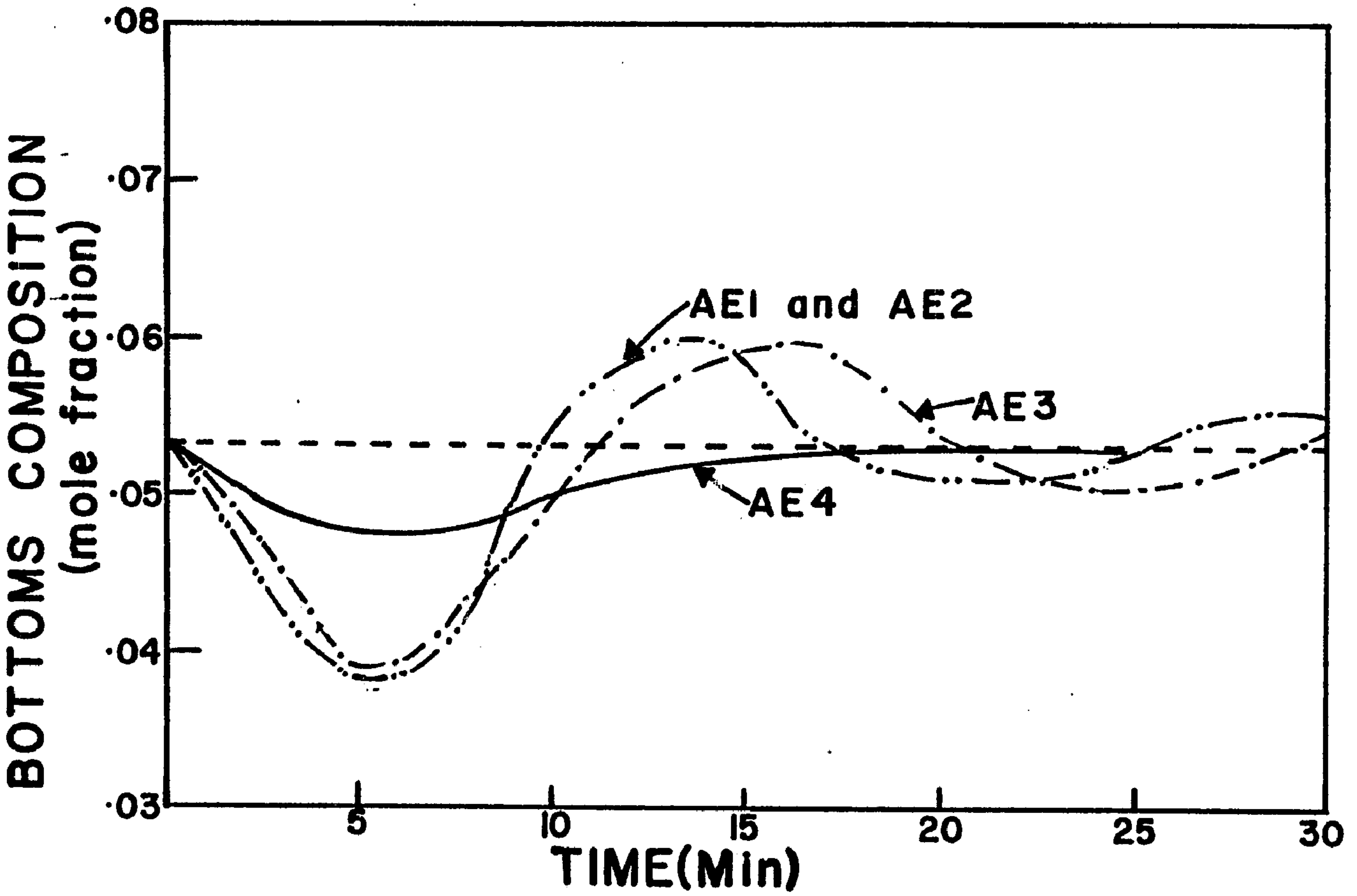


Figure 34. Bottom's Product Composition Response for Approximate Estimator Based Dual Composition Control Schemes for a Step Change in Feed Composition.

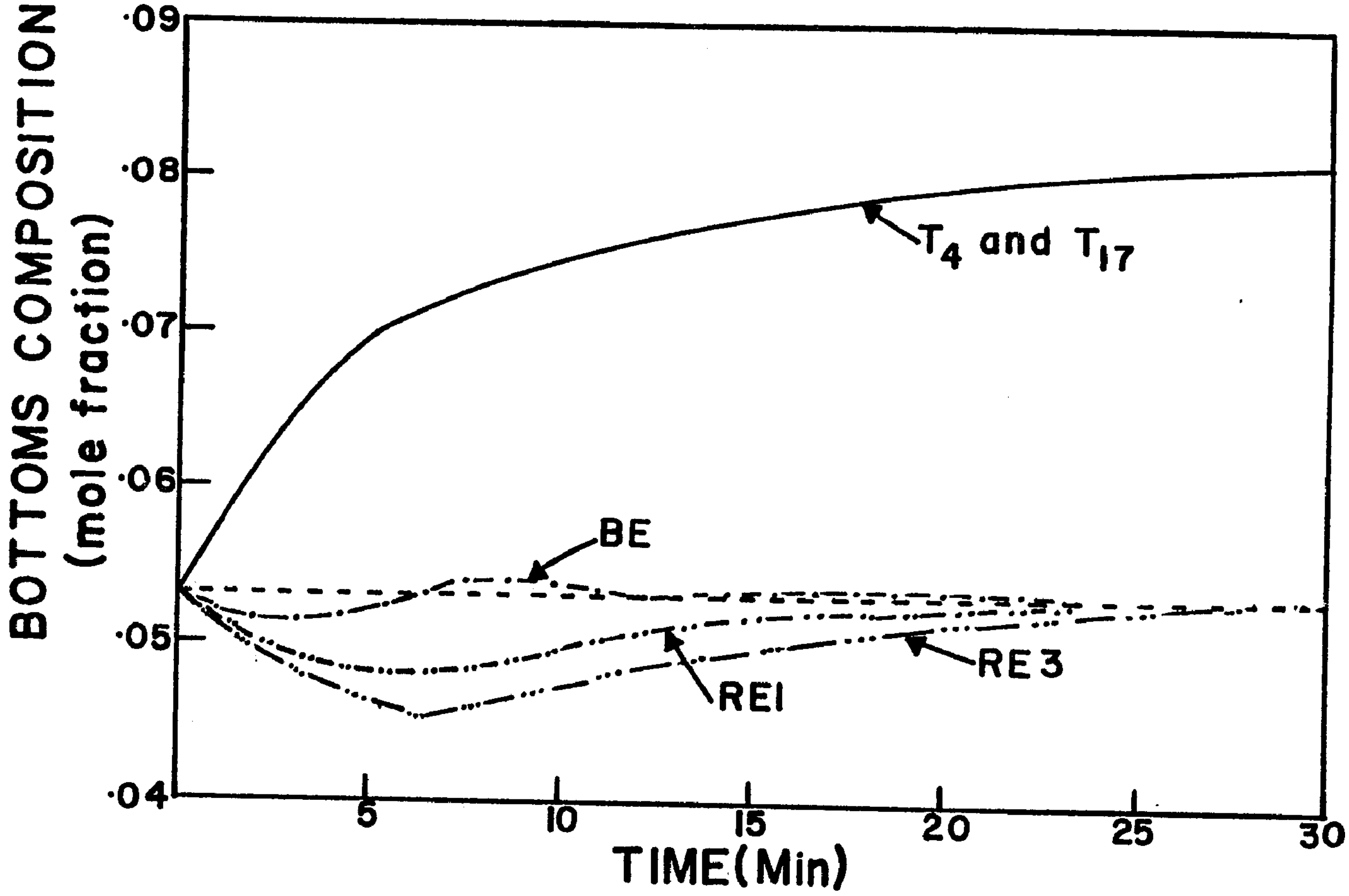


Figure 35. Bottom's Product Composition Responses for Dual Composition Control Schemes for a Step Change in Feed Composition

Table 8. Process Transfer Functions with Respect to Reflux Flow Rate and Controller Settings for Top Control Loops (Dual Composition Control)

Control Scheme	Process Variable	Transfer Function	Controller Settings	
			Gain**	Reset Time (min)
Controlling Tray 4 and Tray 17 Temperatures	Tray 17 Temperature	$\frac{-.57e^{-.7S}}{(6S+1)}\ \frac{^{o}\text{C}}{\text{gmole/min}}$	1.044	1.73
	Tray 4 Temperature	$\frac{-.37e^{-.78S}}{(5.5S+1)}\ \frac{^{o}\text{C}}{\text{gmole/min}}$		
Brosilow's Linear Estimator	Estimated Distillate Composition	$\frac{.0053e^{-.65S}}{(6S+1)}\ \frac{\text{mole fraction}}{\text{gmole/min}}$	180.	1.88
	Estimated Bottom's Composition	$\frac{.0093e^{-.85S}}{(6.2S+1)}\ \frac{\text{mole fraction}}{\text{gmole/min}}$		
*AE1 Estimator, 2nd order		$\frac{-6.95e^{-.4S}}{(5S+1)} - .38\ \frac{^{o}\text{C}}{\text{gmole/min}}$	.48	0.5
*AE2 Estimator, 2nd order		$\frac{-1.47e^{-.1S}}{(4.6S+1)} -1\ \frac{\text{gmole/min}}{\text{gmole/min}}$	1.35	0.5
*AE3 Estimator, 2nd order		$\frac{1.62e^{-.02S}}{(5.2S+1)}\ \frac{\text{gmole/min}}{\text{gmole/min}}$	.12	0.5
*AE4 Estimator, Three Temperatures		$\frac{2.23e^{-.3S}}{(5.3S+1)}\ \frac{^{o}\text{C}}{\text{gmole/min}}$	.48	0.5
RE1 Estimator	Estimated Distillate Composition		360.	0.5
RE3 Estimator	" "		180.	0.75

*As defined in Table 3.
**The units are reciprocal of the units for the corresponding transfer function.

Table 9. Process Transfer Functions with Respect to Steam Flow Rate and Controller Settings for Bottom Control Loop (Dual Composition Control)

Control Scheme	Process Variable	Transfer Function	Controller Settings Gain*	Controller Settings Reset Time (min)
Controlling Tray 4 and Tray 17 Temperatures	Tray 4 Temperature	$\frac{.457\, e^{-.1S}}{(5.2S+1)}\ \frac{^{o}C}{g\text{-mole/min}}$	.202	0.5
	Tray 17 Temperature	$\frac{.405 e^{-.15S}}{(5.6S+1)}\ \frac{^{o}C}{g\text{-mole/min}}$		
Brosilow's Linear	Estimated Bottom's Composition	$\frac{.013\, e^{-.02S}}{(5.9S+1)}\ \frac{\text{mole fraction}}{g\text{-mole/min}}$	10.8	0.5
	Estimated Distillate Composition	$\frac{.0035 e^{-.25S}}{(5.6S+1)}\ \frac{\text{mole fraction}}{g\text{-mole/min}}$		
RE1 Estimator	" "		50.4	.5
RE3 Estimator	" "		50.4	.8

*The units are reciprocal of the units for the corresponding transfer function.

The control achieved by estimator based control schemes is more stable than the control achieved by controlling two tray temperatures. The steady state composition errors in face of feed composition disturbances are almost nonexistent for estimator based control schemes.

8. DESCRIPTION OF THE EXPERIMENTAL SYSTEM

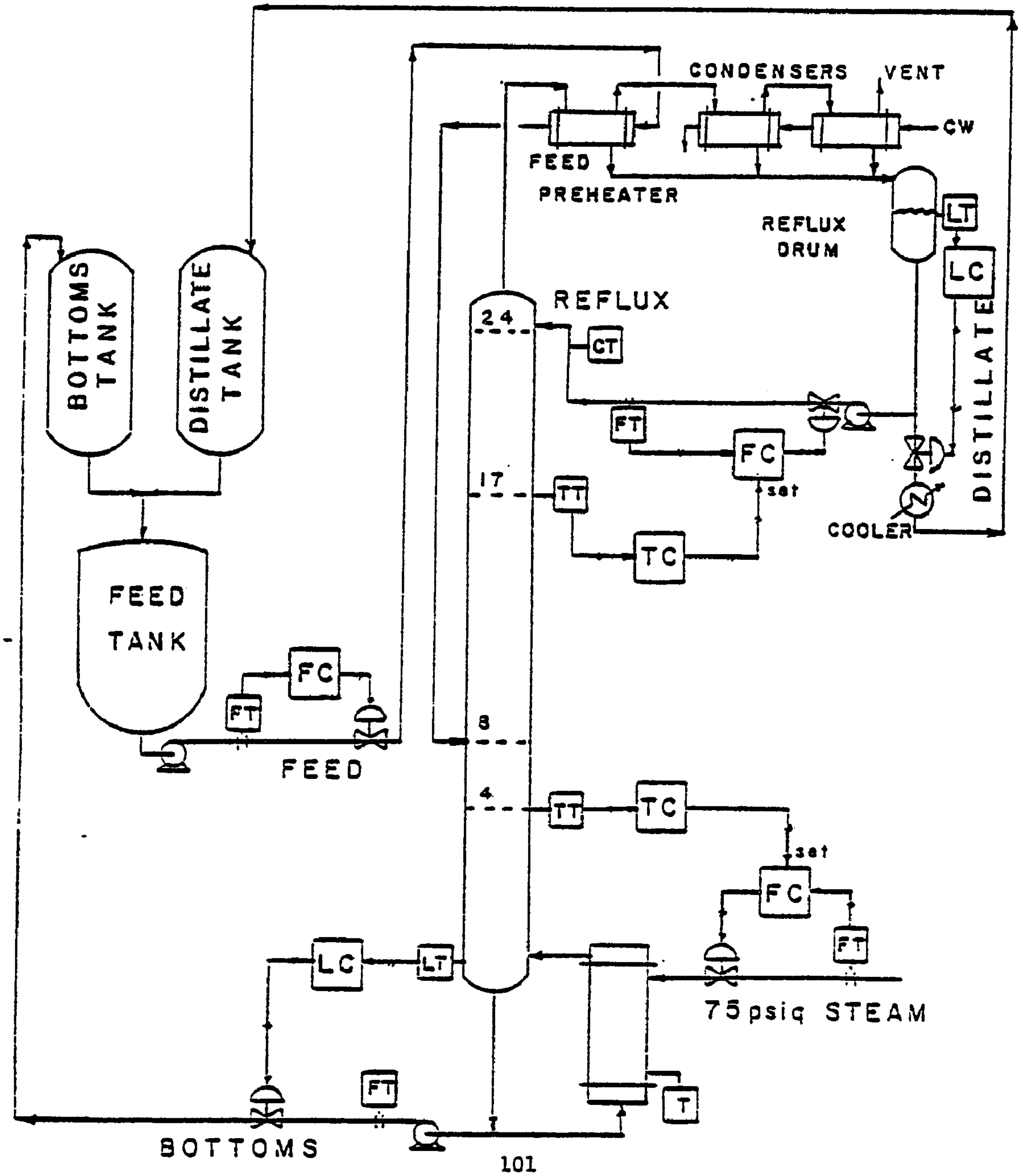
The experimental setup consisted of a distillation unit interfaced with a PDP 11/40 computer. The distillation column was a pilot scale, 24 tray, 8" I.D. column separating methanol/water mixture at atmospheric pressure. The trays were bubble cap trays separated by six inches. The column is equipped with a vertical thermosyphon reboiler, feed preheater, overhead total condenser and a reflux drum. Figure 36 shows the distillation column with basic feedback control loops.

The product compositions were controlled by cascade control of tray 17 and tray 4. Two pneumatic temperature transmitters were used to measure the temperatures. The pneumatic cascade controllers were capable of controlling a tray temperature, the process flow rate or the valve position. The distillate composition is continuously monitored by a Princo Densitrol. The process flow rates were measured with pneumatic integral orifice /differential pressure flow transmitters. Thermocouples were used to measure six tray temperatures, feed temperature and reflux temperature, which were recorded on a multipoint temperature recorder. Four process flow rates (reflux, distillate, steam and bottom's), distillate composition and bottom's level were continuously recorded.

The DEC PDP 11/40 computer used in this study has 16K core memory and moving head RK11 disk. The peripheral

Figure 36

LEHIGH DISTILLATION COLUMN



devices include decwriter, card reader and high speed paper tape reader and punch. It has 32 analog input channels and four analog output channels. The computer uses DOS/BATCH monitor operating system. RSX11-B was the real time executive.

Twelve pneumatic signals (3-15 psig) from the column were converted to voltage signals (0-10 volts) using P/V transducers. Twelve thermocouple millivolts signals were (Fe/CO thermocouple, range $10^{o}C$ to $110^{o}C$) converted to voltage signals (0-10V) by millivolt/voltage transducers. These analog voltage signals were fed to the A/D converter which was scanned by the computer. The computer sends analog voltage signals (0-10V) from D/A converters to V/P transducers which convert these signals to pneumatic signals (3-15 psig). Available instrumentation permits easy switch over from pneumatic control to computer control of two cascade control loops and two level control loops. In case of cascade control loops, master control loop is put on sample data control and the setpoint signals are sent to pneumatic flow controllers.

9. EXPERIMENTAL RESULTS

The experimental system was tested for bottom's product composition setpoint changes for i) RE1 estimator based control scheme, ii) Brosilow's linear estimator based control scheme.

It was shown by simulation studies that the rigorous estimator based control schemes had a clear advantage over Brosilow's linear estimator based control scheme for bottom's product composition setpoint changes. The latter control scheme showed large steady state product composition deviations. The objective for the experimental study was to verify these simulation results and actually test the feasibility of estimator based control schemes on the experimental system.

The reflux flow rate and steam flow rate were maintained constant by flow control until steady state was attained. A bottom's product composition setpoint step disturbance from approximately 5 mole percent to .5 mole percent was given. The steam flow rate is manipulated such that the estimated bottom's product composition finally equals 0.5 mole percent. The reflux flow rate was maintained constant throughout.

The noise in the secondary process measurements used in these control schemes was filtered using a digital filter with a first order lag of 1 min. The equation representing the digital filter is as follows.

$$x_n = \frac{(2\tau-T)}{(2\tau+T)} \quad X_{n-1} + \frac{T}{(2\tau+T)} \quad (Q_n+Q_{n-1})$$

where

x_n = Digital filter output at $t = nT$

Q_n = Digital filter input at $t = nT$

τ = Digital filter first order lag

T = Sampling period.

For Brosilow's linear estimator, the temperatures of trays 5, 8 and 17 were continuously sampled every ten seconds. The perturbations in the tray temperatures were calculated. The perturbation in the steam flow rate was assumed to be equal to change in steam flow rate setpoint to the flow controller from the steady state value. The initial steady state bottom's product composition was obtained by withdrawing a sample from the line. The estimated bottom's product composition was obtained from the bottom's product composition perturbation calculated from perturbations in tray temperatures and steam flow rate. A sampling period of ten seconds was used. The controller gain of 17.6 $\frac{\text{gmoles/min}}{\text{mole fraction}}$ and reset time 0.5 min. as obtained from simulation studies gave satisfactory dynamic response on the experimental system.

For rigorous estimator, the bottom's product composition, steam flow rate, bottom's flow rate and tray 4 temperature were measured initially at steady state. These initial measurements were adjusted slightly so that they are consistent with steady state model of the column. These are referred to as initialized secondary measurements. The tray 4 temperature and bottom's flow rate were continuously sampled. The perturbations in tray 4 temperature and bottom's flow rate were calculated. The perturbation in steam flow rate was assumed to be equal to the change in steam flow rate set point to the flow controller from the steady state value. The actual value of the secondary measurements were assumed to be equal to the initialized value of the secondary measurements plus the perturbation in the secondary measurements. The bottom's product composition was estimated using RE1 estimator from the actual values of secondary measurements. The program executes within 4K, 16 bit memory. It was found that computer calculation time for RE1 estimator varied from 5 to 25 seconds. Hence, a variable sampling period equal to the computer calculation time plus ten seconds was used in the control algorithm. It was found that the control system was almost undamped when the controller gain of 50.4 $\frac{\text{gmoles/min}}{\text{mole fraction}}$ and reset time of 0.5 min. as obtained from simulation studies were used. The controller gain was reduced to 22.7. This gave a stable, underdamped response.

The experimental results are plotted in Figures 37, 38 and 39. The bottom's product composition was calculated from reboiler temperature. The recorded reboiler

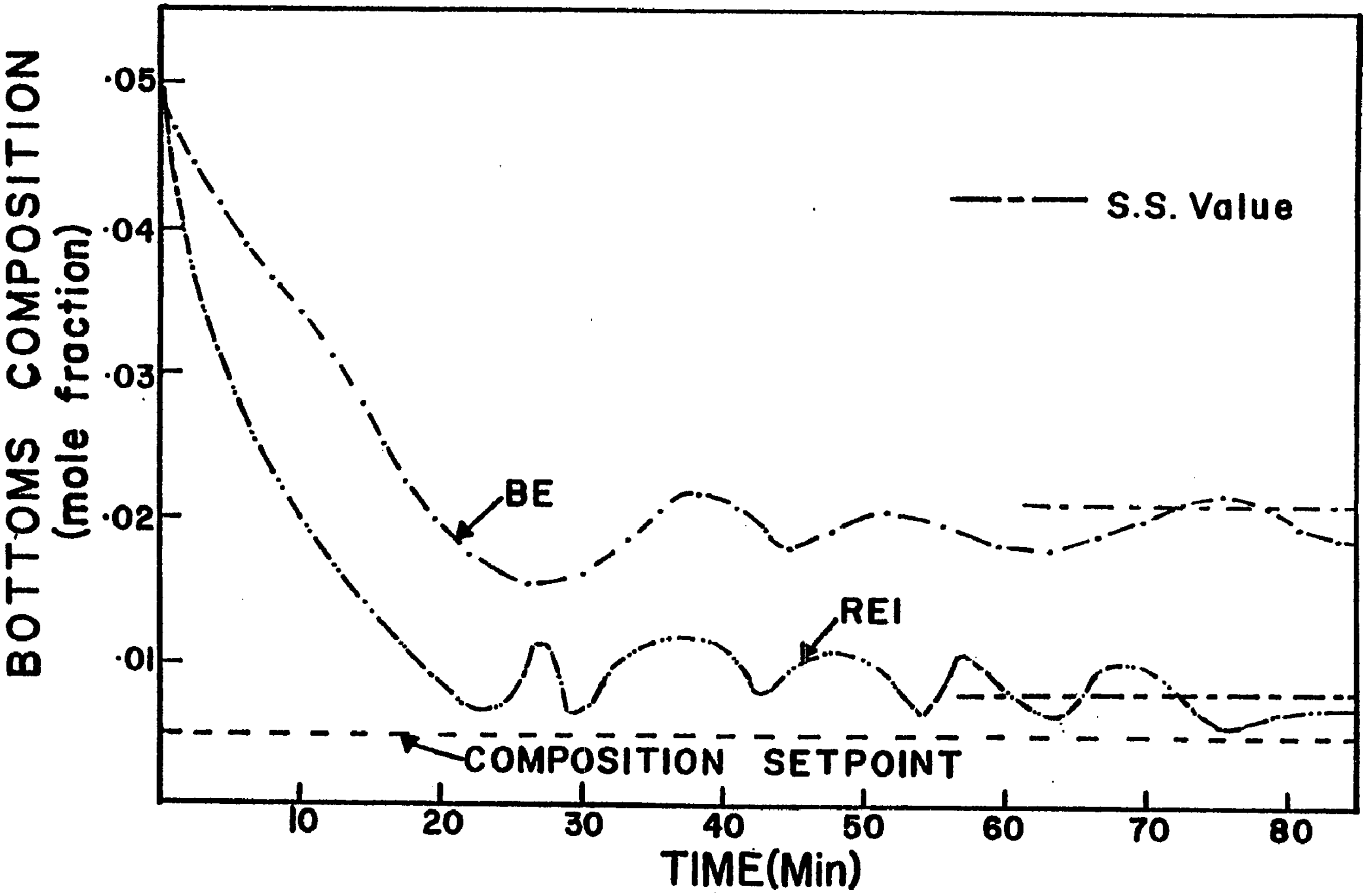


Figure 37. Bottom's Product Composition Response for a Step Change in Bottom's Product Composition Setpoint (Experimental).

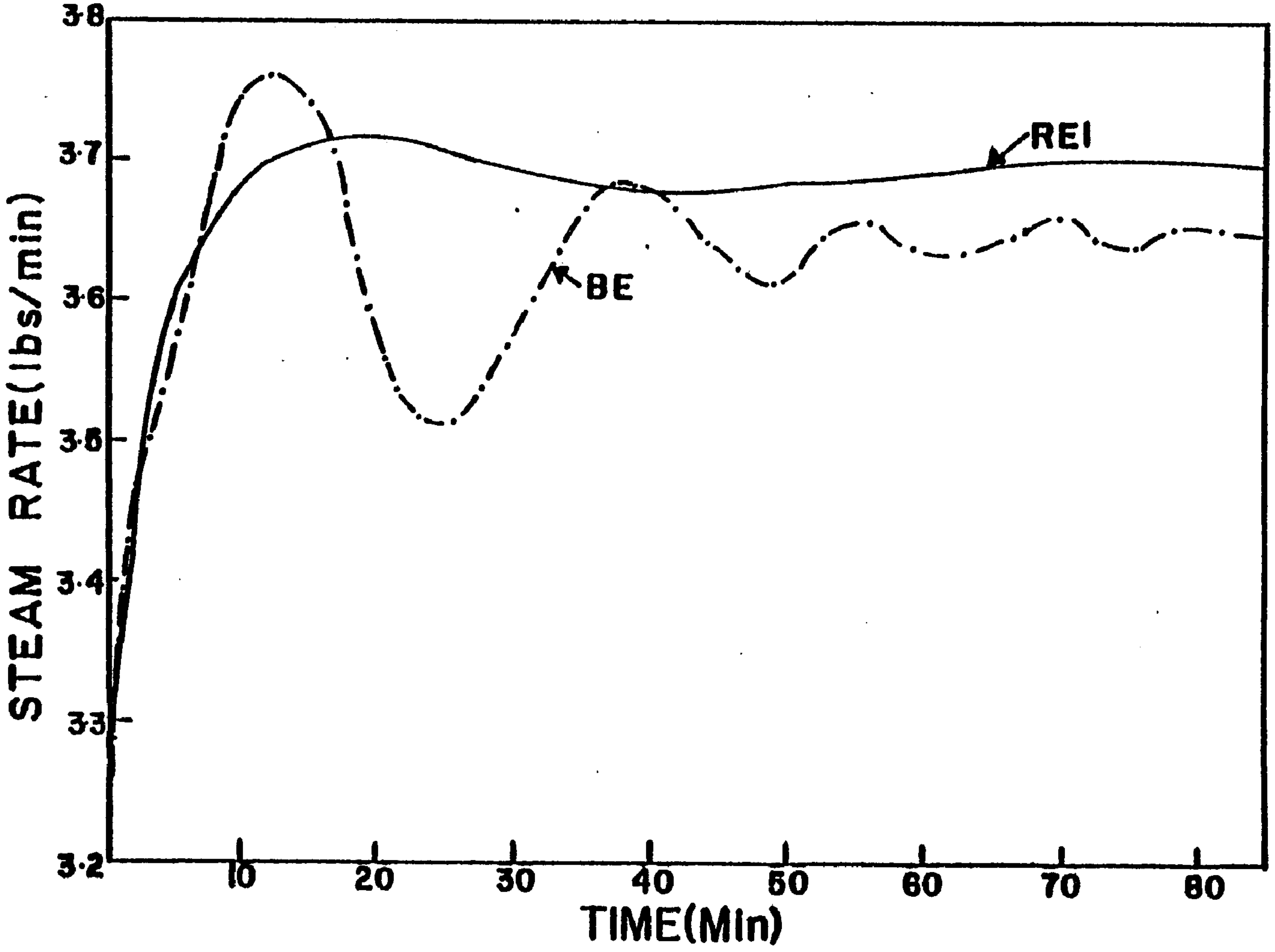


Figure 38. Steam Flow Rate Transient for a Step Change in Bottom's Product Composition Setpoint (Experimental).

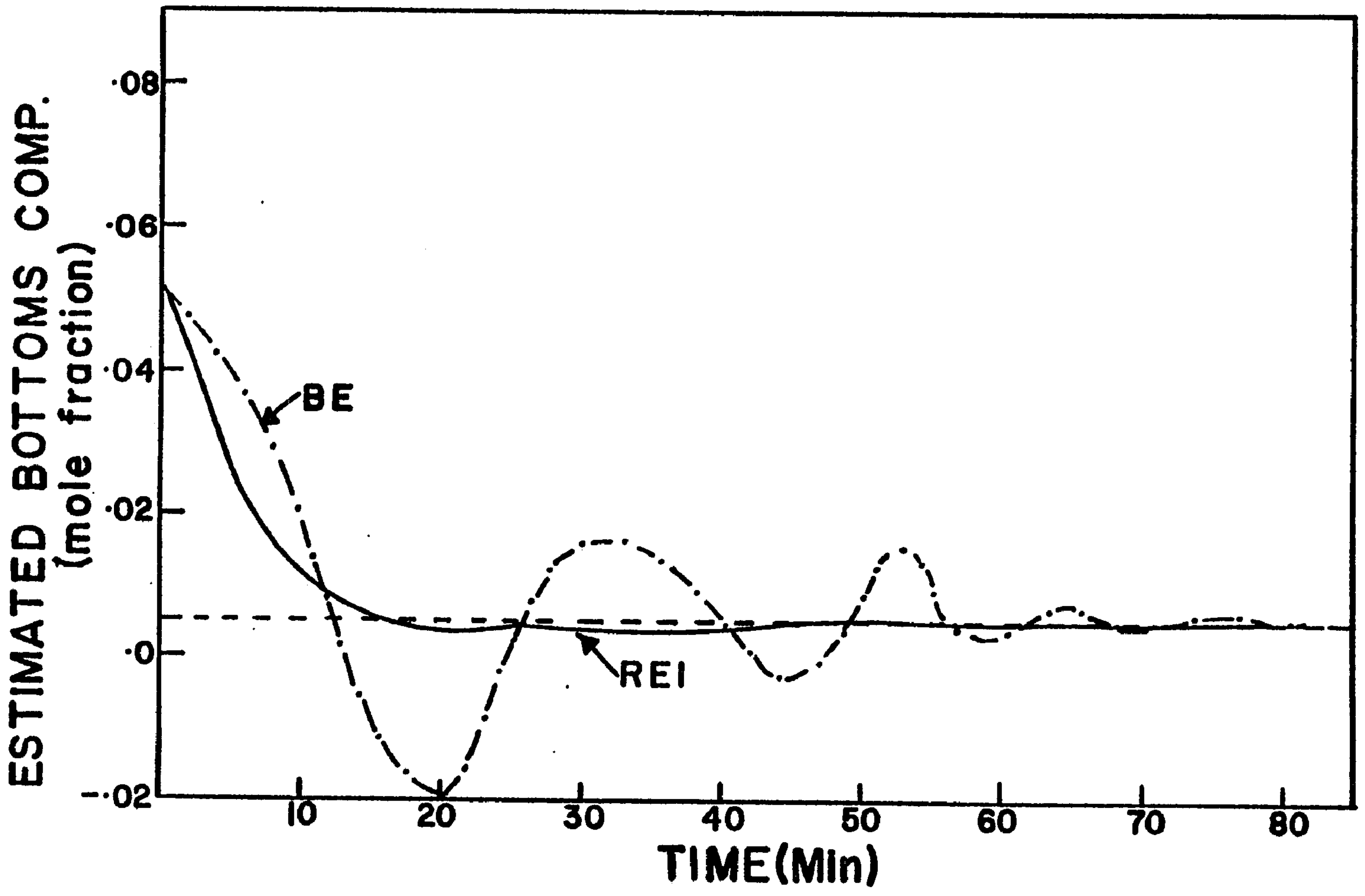


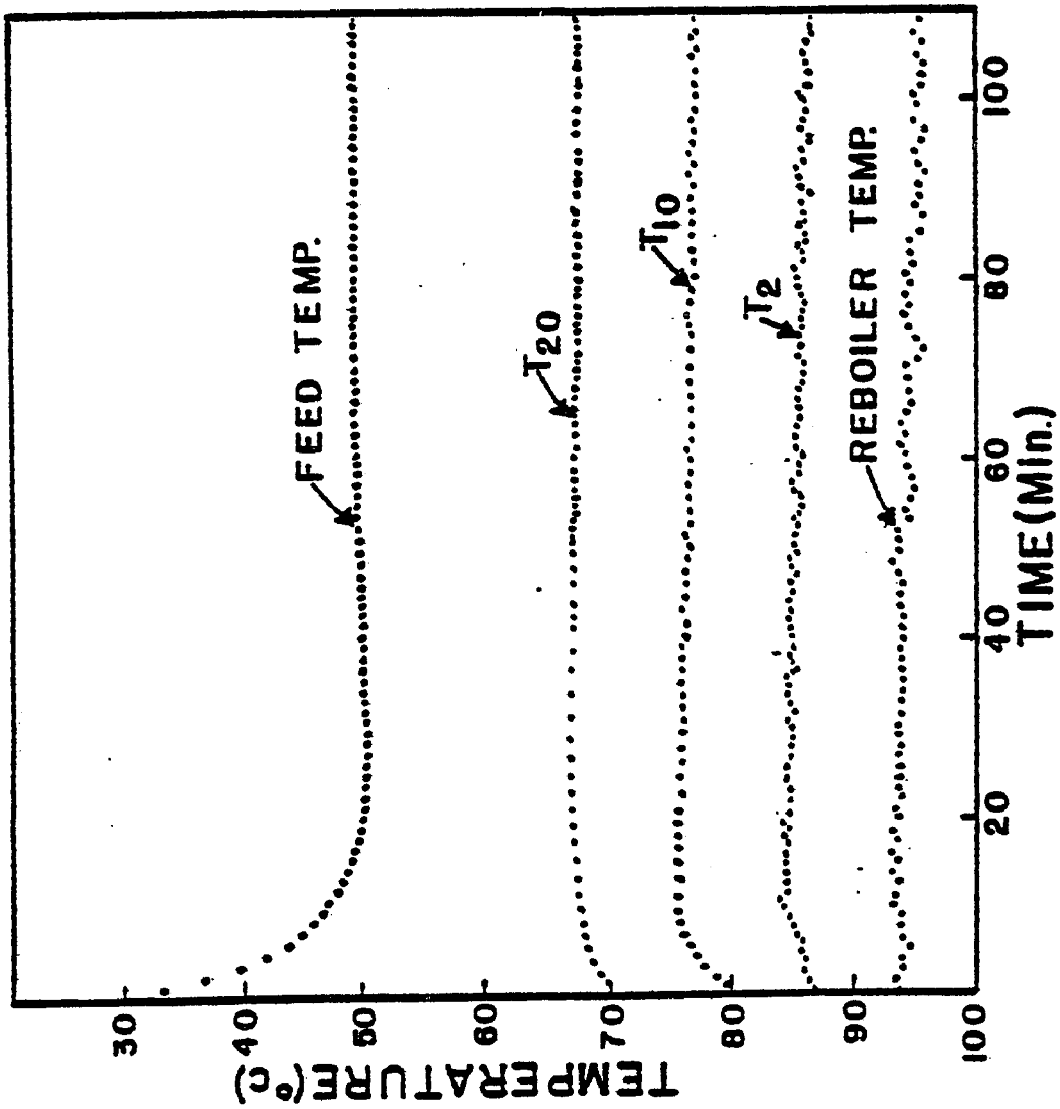
Figure 39. Estimated Bottom's Product Composition Response for a Step Change in Bottom's Product Composition Setpoint.

temperature showed a cyclic, low frequency disturbance as shown in Figure 40. This is reflected in bottom's product composition calculated from the reboiler hold up temperature.

The sampled-data control programs for both control schemes are given in Appendix D. The final steady state bottom's product composition for both control schemes was obtained by withdrawing a sample from the line. The final bottom's product composition of 2.1 percent was obtained for Brosilow's linear estimator and 0.8 percent was obtained for RE1 estimator.

The experimental results essentially reinforce the simulation results which showed that rigorous estimator based control scheme was more stable and had a smaller steady state composition error for change in bottom's product composition set point compared to Brosilow's linear estimator based control scheme. Theoretically, rigorous estimator based control scheme should not show any steady state product composition error. However, the steady state composition error of 0.3 percent observed experimentally can be attributed to change in column parameters and experimental inaccuracies.

Figure 40. Reboiler Holdup Temperature Disturbance (Startup of the Column).



10. DISCUSSION AND CONCLUSION

The composition control achieved by using estimator based composition control schemes is superior to that achieved with conventional control schemes.

For the particular experimental system studied, the performance of the control scheme based on Brosilow's linear estimator was satisfactory in face of feed composition and distillate composition set point disturbances. However, it showed large steady state composition deviations for bottom's product composition set point disturbances. Such a control scheme is likely to give large steady state product composition errors for a nonlinear system subject to large load disturbances. Besides, Brosilow's linear estimators have to be reconstructed if column parameters change significantly.

Control schemes based on approximate estimators performed satisfactorily in face of feed composition disturbances. Approximate estimators are designed to handle column nonlinearities in face of feed composition changes. However, they are less flexible in the sense that no composition set point changes can be given. Also, the approximate estimators have to be reconstructed if the column parameters change significantly.

The control schemes based on rigorous estimators (RE1 and RE3) performed satisfactorily in face of feed composition or set point changes. Rigorous estimators have certain important advantages over other estimators. Since they are based on a fundamental steady state distillation column model, they are better suited to handle column nonlinearities. They are easy to implement and to modify if column parameters change. One important drawback is large amount of computations required. However, this should not be a serious problem considering the sophistication of modern control computers. RE3 rigorous estimator would perform better than RE1 rigorous estimator when the column temperature profile is likely to change significantly.

There is a predictive feed forward control action associated with estimator based control schemes. This results in a composition control more stable and superior to that attained with instantaneous product composition measurement.

11. RECOMMENDATIONS FOR FURTHER RESEARCH

Feedback control systems are designed using the process transfer functions and/or on line tuning of the controllers. The process is subject to random input disturbances and set point changes. Some system parameters may deviate from the steady state values based on which the control system was designed. Control system performance would deteriorate if these deviations are large, especially if the sensitivity of the control system to these system parameter variations is high.

In case of a distillation column, system parameters like tray efficiencies, tray pressure drop, column heat losses, etc., are subject to variations due to changing environment. This could cause large steady state product composition errors and/or unsatisfactory transient response in face of input disturbances and/or set point changes.

In general, a fruitful area of research would be to modify product composition control strategies to handle changes in column parameters. The first step would be to modify the estimator based control strategies to reduce steady state product composition error in face of column parameter changes.

Brosilow's linear estimator is based on static linear model of the distillation column which relates perturbations in output variables to perturbations in input variables. Finally, perturbation in product composition is expressed as a linear function of perturbations in measurable input disturbances and tray temperatures. The static linear model of the column can be modified to relate perturbations in output variables to perturbations in input variables and important column parameters. (The word "important" is used in the sense that expected variations in this system parameter could cause significant changes in the output variables.) Then, the perturbation in the product composition can be expressed as a linear function of perturbations in measurable input variables and column parameters, and selected tray temperatures.

In case of approximate estimators, the tray temperatures were expressed as a polynomial function of reflux rate/feed rate ratio for a binary column. However, for a binary column subject to parameter variations, the tray temperatures can be expressed as a nonhomogeneous polynomial function of relux rate/feed rate ratio and column parameters. If this polynomial involves n terms, then the function ϕ (as described in AE4 estimator) can be defined as a linear function of n tray temperatures. Indirect composition control is achieved by controlling the value of ϕ.

Compared to other estimators, rigorous estimators possess high degree of flexibility. Tray efficiencies and column heat losses are unmeasurable column parameters subject to change. It was shown that the rigorous estimators are sensitive to tray efficiencies and relatively insensitive to changes in tray heat losses.

If three secondary measurements, say two process flow rates and a tray temperature, are known, the produce composition in that section can be estimated. Now, if tray efficiency in the section is not known, the degree of freedom of the system is reduced by one. Knowledge of one additional tray temperature completely specifies the system.

The rigorous estimators would involve two dimensional search to determine a set of values of tray efficiency and produce composition that satisfy the two temperatures and two flow rates measured.

One way to accomplish this is to guess the value of tray efficiency in the section. The estimated produce composition for one tray temperature is calculated as described in RE1 estimator. Similarly, another product composition estimate for another tray temperature is obtained. The difference between the two composition estimates is compared and a new value of tray efficiency is guessed. This procedure is repeated, using interval-halving search method to determine the tray efficiency for which the difference between the two composition estimates is less than the error criterion. Although this technique is worth investigation, it is likely to run into trouble because of column dynamics. This technique is referred to as modified RE1 estimator.

Another technique is based on RE3 estimator which involves one dimensional search to determine product composition for which the summation of the squares of differences between calculated and recorded tray temperatures is minimised. This is based on the assumption that the tray efficiency in the section is known. Assuming the tray efficiency is not known, a two dimensional search can be made to determine a set of values of tray efficiency and product composition which minimises the sum of square of difference between recorded and calculated tray temperatures. This technique is less likely to run into difficulty due to column dynamics. This is referred to as modified RE3 estimator.

Both the above mentioned modified rigorous estimator techniques are expected to require a large amount of computations. In certain cases, it may be advisable to develop a real time task which, after verifying that the column is at steady state, calculates tray efficiency in the section using one of the two modified rigorous estimators at specified interval of time or at operator's command. Then the tray efficiency is updated in another real time task which controls product composition using a rigorous estimator.

To obtain satisfactory transient response, the controller settings would have to be continuously adjusted with changing environment. This can be best accomplished by an adaptive control scheme.

Another area of fruitful research would be to extend rigorous estimators to multicomponent columns.

Consider a multicomponent column with n components. Theoretically, if at least (n-1) tray temperatures and two process flow rates are known in a section of the column, the product composition in that section is fixed. Conversely, if the product composition and two process flow rates are known in a section of the column, the temperature profile in that section of the column can be constructed. The computational procedure similar to that used for modified RE1 and RE3 estimators can be used to determine product composition. However, (n-1)th dimensional search would be necessary to determine product compositions. This could get computationally complex and time consuming for a column with a large number of components. Some simplifying assumptions based on individual nature of the column might be necessary.

APPENDIX A

PHYSICAL DATA

Enthalpy

Vapor Phase $\mathrm{ENTV} = 11440 - 1990\ Y$ (cals/gmole)

Liquid Phase $\mathrm{ENTL} - 1800 - 2433\ X + 1753\ X^2$ (cals/gmole)

Specific Heats

Water

$CP_W = 18.016$ cals/gmole

Methanol

$CP_M = 22.4$ cals/gmole

Density-Temperature Relation

Water

$$\rho_W = 1.00523 - 2.135 \times 10^{-4} \times t - 2.55 \times 10^{-6} \times t^2 \quad \text{(gm/cc)}$$

Methanol

$$\rho_M = 0.8099 - 9.253 \times 10^{-4} \times t - 7 \times 10^{-7} \times t^2 \quad \text{(gm/cc)}$$

where

t is temperature in °C.

Vapor Pressure

Expressed as

$$\ell n\ P_i = \frac{A_i}{T} + B_i$$

Water

$A_2 = -4981.036$

$B_2 = 13.3486$

Methanol

A_1 = -4386.934

B_1 = 12.9848

where

p is in atmospheres and T is in ^{o}K.

Vapor-Liquid Equilibrium

The equilibrium vapor composition is calculated from liquid composition by calculating activity coefficient using Van-Larr equations.

$$\ell n\ \gamma_1 = \frac{A_1}{(1 + \frac{A_1}{B_1} \cdot \frac{X_1}{X_2})^2}$$

$$\ell n\ \gamma_2 = \frac{B_1}{(1 + \frac{B_1}{A_1} \cdot \frac{X_2}{X_1})^2}$$

where

A_1 = 0.9

B_1 = 0.48

X_1 = Mole fraction of methanol

X_2 = Mole fraction of water

γ_1 = Activity coefficient for methanol

γ_2 = Activity coefficient for water

APPENDIX B

RIGOROUS ESTIMATORS

A. Steady State Equations

A representative binary column with one feed and no side streams is shown in figure B-1.

Overall material balance around envelope 1

$$V_n = L_{n+1} + D \tag{1}$$

Component material balance around envelope 1

$$V_n \cdot Y_n = L_{n+1} \cdot x_{n+1} + D \cdot x_D \tag{2}$$

Energy balance around envelope 1

$$V_n \cdot H_n = L_{n+1} \cdot h_{n+1} + D \cdot h_D + Q_C + (NT-n) \cdot QL \tag{3}$$

From Eq. (1), Eq. (2), and Eq. (3)

$$Y_n = x_{n+1} + \frac{(H_n - h_{n+1})(x_D - x_{n+1})}{\left(\frac{QC + (NT-n) \cdot QL}{D} - h_{n+1} + h_D\right)} \tag{4}$$

Condenser material balance

$$V_{NT} = R + D \tag{5}$$

Condenser energy balance

$$V_{NT} \cdot H_{NT} = (R + D) \cdot h_D + Q_C \tag{6}$$

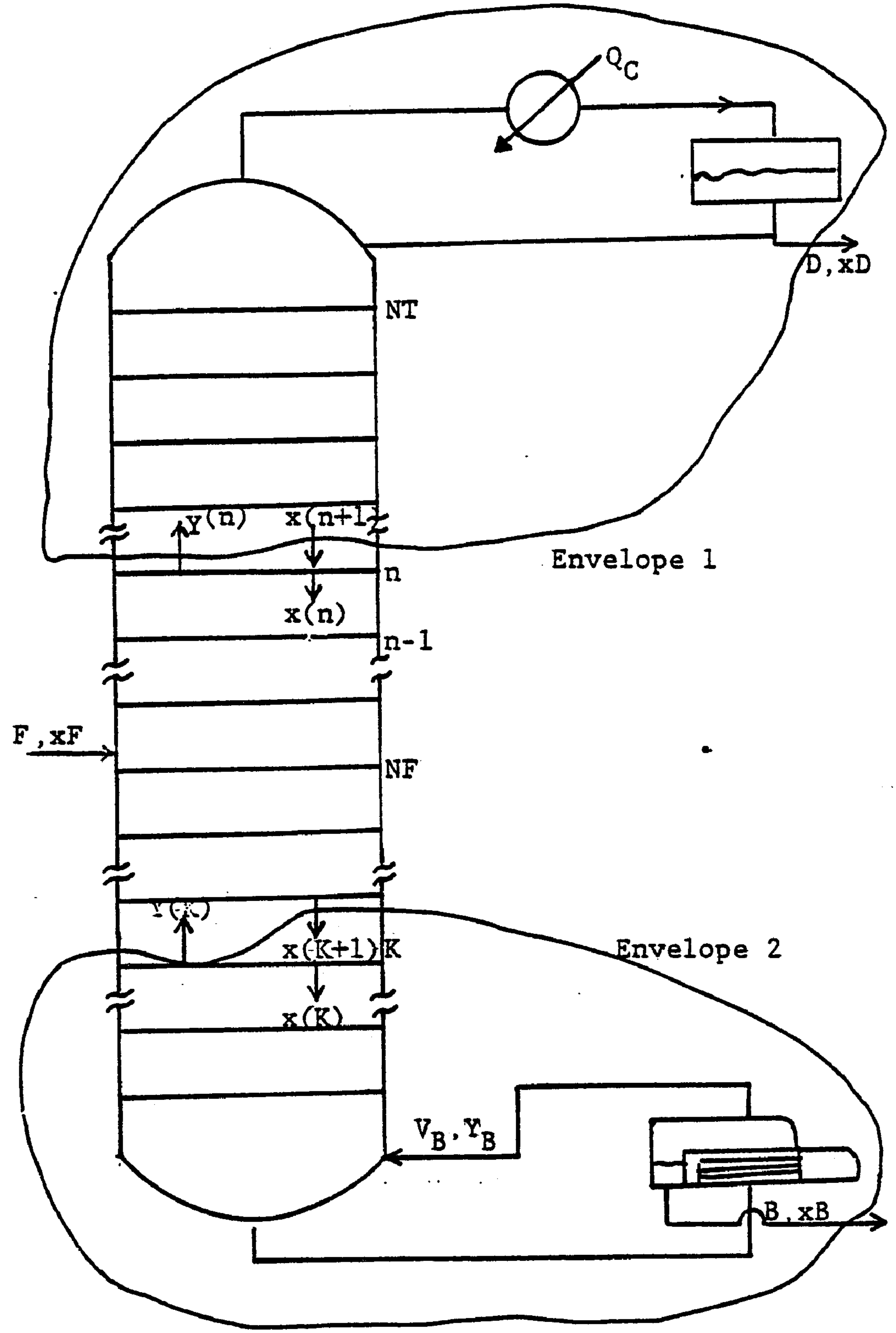
From Eq. (5) and Eq. (6)

$$Q_C = (R+D)(H_{NT} - h_D) \tag{7}$$

Murphree Efficiency in rectifying section

$$EFFR = \frac{Y_n - Y_{n-1}}{Y_n^* - Y_{n-1}} \tag{8}$$

Figure B-1. Binary Distillation Column.



On simplifying Eq. (8)

$$Y_n = (1 - EFFR) \cdot Y_{n-1} + EFFR \cdot Y_n^* \tag{9}$$

Overall material balance around envelope 2

$$V_K = L_{K-1} - B \tag{10}$$

Component material balance around envelope 2

$$V_K \cdot Y_K = L_{K+1} \cdot x_{K+1} - B \cdot x_B \tag{11}$$

Energy balance around envelope 2

$$V_K \cdot H_K = L_{K+1} \cdot h_{K+1} - B \cdot h_B + Q_B - (K) \cdot QL \tag{12}$$

from Eq. (10, Eq. (11) and Eq. (12)

$$Y_K = x_{K+1} + \frac{(H_K - h_{K+1})(X_{K+1} - X_B)}{(\frac{Q_B - (K) \cdot QL}{B} + h_{K+1} - h_B)} \tag{13}$$

Eq. (13) can be simplified for reboiler

$$Y_B = x_1 + \frac{(H_B - h_1)(x_1 - x_B)}{(\frac{Q_B}{B} + h_1 - h_B)} \tag{14}$$

Murphree efficiency in the stripping section.

$$EFFS = \frac{(Y_K - Y_{K-1})}{(Y_K^* - Y_{K-1})} \tag{15}$$

Eq. (15) can be simplified to

$$Y_K = (1 - EFFS) \cdot Y_{K-1} + EFFS \cdot Y_K^* \tag{16}$$

Murphree efficiency for the reboiler gives

$$Y_B = (1-EFFS) \cdot X_B + EFFS \cdot Y_B^* \tag{17}$$

B. Distillate Composition Estimation

B-1. RE1 Rigorous Estimator

If 1) rectifying section tray efficiency, 2) tray pressures, 3) tray heat losses, and 4) reflux temperature are known, then reflux rate, distillate rate and a tray temperature (i^{th} tray) in rectifying section are required to estimate the distillate composition.

1) Using i^{th} tray temperature, calculate x_i using equilibrium data.

2) Make an initial guess for x_D.

3) Calculate condenser heat load using Eq. (7).

4) Since x_i is known, Y_{i-1} can be calculated using Eq. (4) by trial and error.

5) Calculate Y_i using Eq. (9).

6) Since Y_i is known, x_{i+1} can be calculated using Eq. (4) by trial and error.

7) Calculate Y_{i+1} using Eq. (9).

8) Repeat steps 6) and 7) working up the column until Y_{24} is computed.

9) Compare the calculated Y_{24} with the guessed x_D. If the difference is larger than the error criterion, make another guess for x_D using interval having technique.

10) Repeat steps 3) to 9) until the difference between calculated Y_{24} and x_D is less than the error criterion.

B-2. RE3 Rigorous Estimator

It is assumed that reflux rate, distillate rate and a number of tray temperatures in the rectifying section are known.

1) Make an initial guess for x_D.

2) Make an initial guess for x_{NF+1}, and calculate Y_{24} by the procedure described in RE1 estimator (steps 4) to 8)).

3) If the difference between calculated Y_{24} and x_D is greater than the error criterion, make another guess for x_{NF+1}, and repeat the procedure until the difference between calculated Y_{24} and x_D is less than the error criterion.

4) Calculate ψ, defined as the sum of squares of differences between calculated tray temperatures and measured tray temperatures.

5) Guess a new value of x_D and repeat steps 2) to 4), if the difference between two successive values of ψ is greater than the error criterion.

6) Repeat the procedure using interval halving technique, until the difference between two successive values of ψ is less than the error criterion. (The objective is to determine the value of x_D which minimizes ψ.)

C. Bottom's Product Composition Estimation

C-1. RE1 Rigorous Estimator

If 1) stripping section tray efficiency, 2) reboiler heat loss, 3) tray heat losses, and 4) tray pressures are known, the bottom's product composition can be estimated from the knowledge of steam flow rate, bottom's flow rate and a tray temperature (j^{th} tray) in the stripping section.

1) Calculate the effective heat input Q_B using steam rate and reboiler heat loss.

2) Make an initial guess for x_B.

3) Calculate Y_B using Eq. (17).

4) Calculate x_1 using Eq. (14), since Y_B is known.

5) Calculate Y_1, using Eq. (16).

6) Calculate x_2 using Eq. (13), since Y_1 is known.

7) Repeat steps 5) and 6) working up the column, till x_j is calculated.

8) Calculate j^{th} tray temperature from x_j using equilibrium relationship.

9) If the calculated and recorded value of j^{th} tray temperature differs more than the error criterion, make a new guess for x_B.

10) Repeat the procedure, till the difference between calculated and recorded values of j^{th} tray temperature is less than the error criterion.

C-2. RE3 Rigorous Estimator

It is assumed that steam flow rate, bottom's flow rate and a number of stripping section tray temperatures are known.

1) Calculate the effective heat input Q_B using

steam flow rate and reboiler heat loss.

2) Make an initial guess for x_B.

3) Following the procedure described in RE1 rigorous estimator (steps 3) to 8)), the tray temperatures in the stripping section can be calculated.

4) Calculate ψ, defined as the sum of squares of differences between calculated and recorded tray temperatures and guess a new value for x_B if two successive values of ψ differ more than the error criterion using interval halving technique.

5) Repeat the procedure using interval halving technique, until two successive values of ψ differ less than the error criterion. The objective is to determine the value of x_B which minimizes ψ.

APPENDIX C

A. Experimental Data (Steady State No. 1)

Average operating conditions for Steady State No. 1 are given.

Feed rate = 110.13 gmoles per minute.

Distillate rate = 40.26 gmoles per minute.

Reflux rate = 40.80 gmoles per minute.

Bottom's rate = 69.32 gmoles per minute

Steam rate = 2.96 pounds per minute.

Distillate composition = 96.6 mole percent methanol.

Bottom's product composition = 5.3 mole percent methanol

Feed composition = 39.1 mole percent methanol

Reflux temperature = 49 degrees Celsius

Feed temperature = 60 degrees Celsius

Inlet steam pressure = 75 psig

Calandria steam pressure = 15 psig

Column pressure drop = 51 cms of water

Column base pressure = 1.5 psig

Stripping section tray efficiency = 40 percent

Rectifying section tray efficiency = 51 percent

Feed tray = 8

Reboiler holdup = 11.75 litres

Reflux drum holdup = 6.05 litres

Reflux piping holdup = 1.33 litres

B. Experimental Data (Steady State No. 2)

Feed rate = .308 gallons per minute
= 134.68 gmoles per minute

Reflux rate = .44 gallons per minute
= 40.6 gmoles per minute

Distillate rate = .465 gallons per minute
= 34.7 gmoles per minute

Bottom's rate = .53 gallons per minute
= 106.3 gmoles per minute

Steam rate = 1.47 kg per minute

Cooling water rate = 26 litres per minute

Feed composition = 27.8 mole percent methanol

Distillate composition = 97.7 mole percent methanol

Bottom's composition = 4.3 mole percent methanol

Feed temperature = 60 degrees Celsius

Reflux temperature = 49 degrees Celsius

Cooling water inlet temperature = 7 degrees Celsius

Cooling water outlet temperature = 30 degrees Celsius

Inlet steam pressure = 75 psig

Calandria steam pressure = 20 psig

Column base pressure = 1.35 psig

Column pressure drop = 45.8 cms of water

Feed tray = 8

Reboiler holdup = 11.75 litres

Reflux drum holdup = 6.05 litres

Reflux piping holdup = 1.33 litres

C. Material Balances

To make the overall mass and component material balances exact, the flow rates were slightly adjusted assuming the composition measurements are accurate. The adjusted flow rates are as follows.

Feed rate = 134.97 gmoles per minute

Reflux rate = 39.8 gmoles per minute

Bottom's rate = 100.97 gmoles per minute

D. Energy Balances

The column energy balance was used to compute the column heat losses.

Energy input to the column
= energy input from the steam stream
+ energy input from the feed stream
= 926.574 kcal per minute

Energy output from the column
= energy output to heat the feed stream
+ energy lost via cooling water
+ energy output via bottom's stream
+ energy output via distillate stream
+ heat losses
= 805.872 + heat losses

Total heat losses = 120.702 kcal per minute

Energy input to the condenser

= energy removed to condense column overhead vapors and subcool to reflux temperature

= 646.446 kcal per minute

Energy output from the condenser

= energy to preheat the feed stream

+ energy lost via the cooling water stream

+ condenser heat loss

= 609.135 + condenser heat loss

Condenser heat loss = 37.311 kcal per minute

Heat losses in the column plus reboiler

= 120.702 - 37.311 = 83.391 kcal per minute

Heat loss in the reboiler was assumed to be 33 percent of heat losses in the column plus reboiler.

E. Column Efficiencies

From the recorded tray temperatures a stripping section tray efficiency of 46.5 percent and rectifying section tray efficiency of 56 percent was obtained.

Variable	Experimental	Calculated
Feed rate	134.68 gmoles/min	134.97 gmoles/min
Distillate rate	34.7 gmoles/min	34.04 gmoles/min
Bottom's rate	106.3 gmoles/min	100.97 gmoles/min
T_2	87.8°C	87.7°C
T_4	83.07°C	83.52°C
T_7	81.14°C	81.1°C
T_8	80.14°C	80.73°C
T_{10}	78.1°C	78.01°C
T_{14}	73.3°C	73.03°C
T_{20}	68.7°C	68.3°C
T_{24}	67.3°C	66.6°C
Reflux rate	40.6 gmoles/min	39.8 gmoles/min

Figure C-1. Steady State Temperature Profile for the Column.

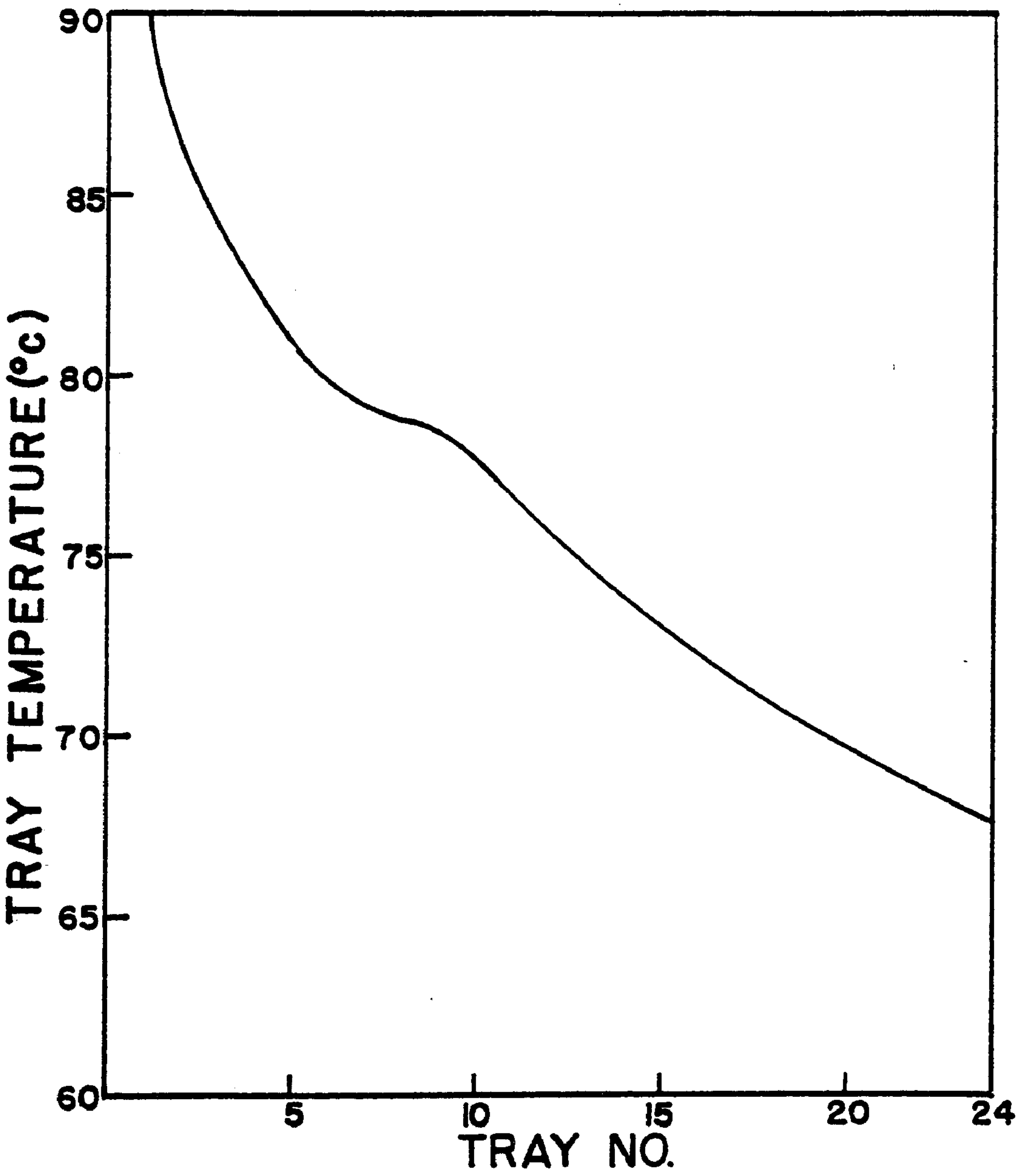
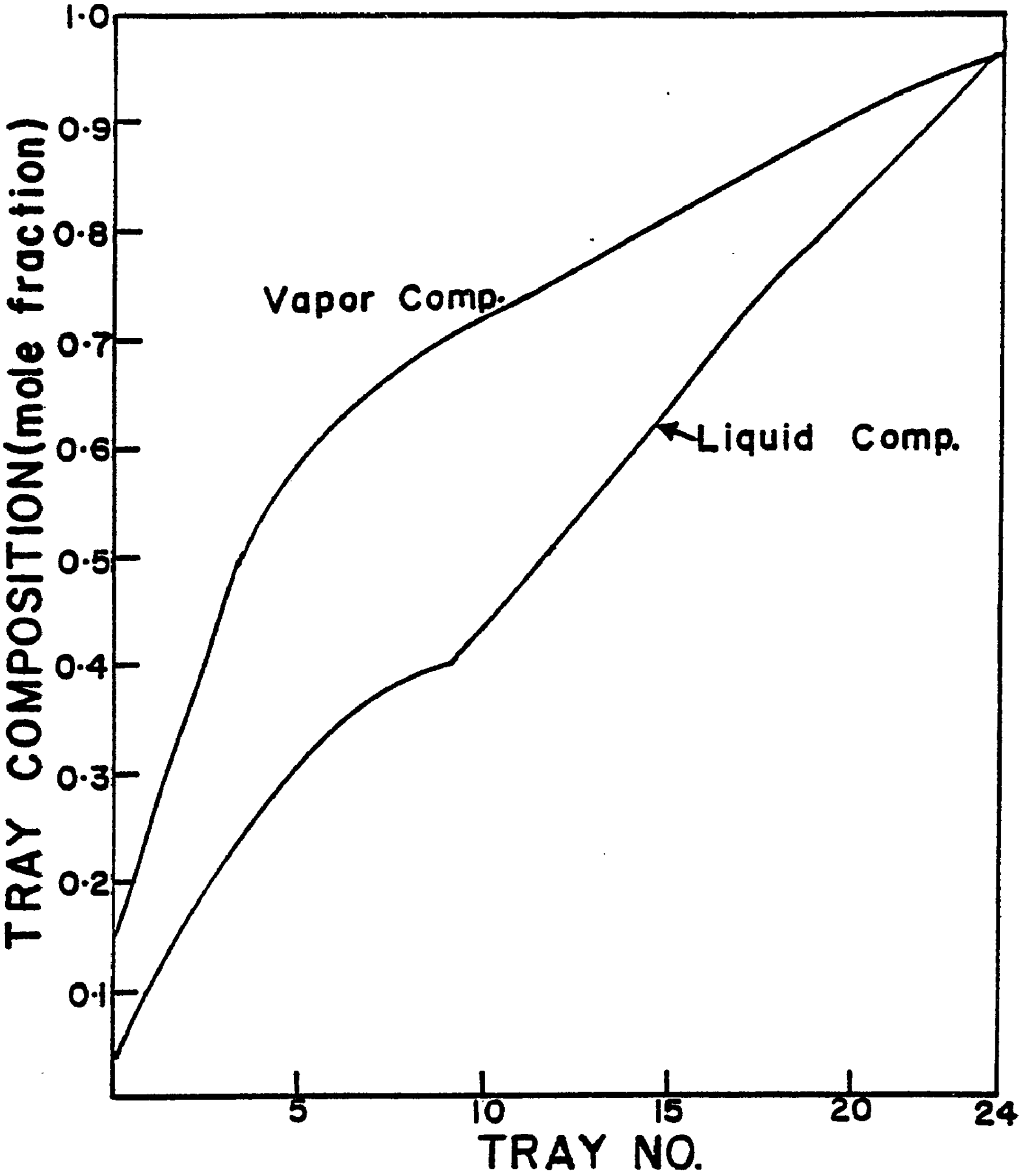


Figure C-2. Steady State Tray Liquid Composition and Vapor Composition Profiles.



APPENDIX D

A. Brosilow's Linear Estimator

```
C...TSK1 performs bottom's composition control using
    Brosilow's linear estimator
    DIMENSION IMULT(3), IN(3), VAR(3), TSET(3), X(3)
    DIMENSION T(3), VOLT(3)
      COMMON/A/XBSET/XB,XKC,TI,TS,SF,T,IP,CALC
C...Temp. tray 5(channel 18), temp. tray 8(channel 15),
C...temp. tray 17(channel 23)
    Data IMULT/18,15,23/
C...Initial data
    ERINT = 0
    XKC = 0.7
    RESET = 30
    IFLAG = 1
    ICOUNT = 1
    IP = 1
    XB = .05
    XBS = XB
    XBSET = .005
    TS1 = 60.
    TS = 10.
C...Brosilow's linear estimator coefficients
    B1 = -.0171193/3.234
    B2 = -.0424033
    B3 = .0387102
```

```
      B4 = .0011154
C...Maintain constant steam flow rate until steady state
      attained.
        SF = 0.77*4.2
      IOUT = 7.7*7.7/10.*204.7
C...Steam flow rate controller setpoint(channel 2)
201     Call AOUT(2,IOUT,IERR)
      ITS = 30
      Call WAIT (ITS,2,IERR)
      IF(IP.EQ.1) GOTO 201
      ITS = TS
C...Scan analog inputs
1     Call AIRDW(3,IMULT,IN,ISTAT)
      do 25 I=1,3
25    VOLT(I) = IN(I)/102.4
      VAR(1) = 10.*VOLT(1)+11.5
      VAR(2) = 10. *VOLT(2)+11.5
      VAR(3) = 50. + 5. *VOLT(3)
      IF(IFLAG.EQ. 1) GO TO 2
C...Digital filtering of input signals
      A1 = (2.*TS1-TS)/(2.*TS1+TS)
      A2 = TS/(2.*TS1+TS)
      T(1) = A1*T(1)+A2*(VAR(1)+X(1))
      T(2) = A1*T(2)+A2*(VAR(2)+X(2))
      T(3) = A1*T(3)+A2*(VAR(3)+X(3))
      GO TO 3
```

```
2   DO 31 I= 1,3
 31   T(I) = VAR(I)
    IFLAG = 2
3   DO 32 1 = 1,3
32    X(I) = VAR(I)
    ICOUNT = ICOUNT+1
    IF(ICOUNT.NE.60) GO TO 4
C...Steady state values of tray temperatures and stem
    flow rate
    DO 33 I = 1,3
33    TSET(I) = T(I)
    SFSET = SF
C...Composition setpoint change given after ten minutes
4   IF(ICOUNT. LT. 61) GO TO 10
C...Estimate bottom's composition
    CALC = B1*(SF-SFSET)+B2*(T(1)-TSET(1))+B3*(T(2)
                                             -TSET(2))
   + B4*(T(3)-TSET(3))
    XB = XBS+CALC
    ERROR = XB-XBSET
    IF(SF.GT.3.78 AND ERROR GT. 0) GO TO 103
    ERINT = ERINT + ERROR*TS*XKC/TI
    SF=SFSET+XKC*ERROR+ERINT
    IF(SF.GT.3.78) GO TO 91
    GO TO 92
91    SF=3.781
```

```
      SFSET=3.781
      ERINT=0.
 92   CONTINUE
        COUT=(SF/4.2)**2*10.
      IF(COUT.GT.10.) COUT=10.
      IOUT=COUT*204.7
C...Steam flow rate controller setpoint(channel 2)
      CALL AOUT(2,IOUT,IER)
 103  CONTINUE
 10   CALL WAIT(ITS,2,IERR)
      GO TO 1
      END
```

B. RE1 Rigorous Estimator

```
C...TSKI performs bottom's composition control using
      RE1 rigorous estimator
      DIMENSION IMULT(2),IN(2),VAR(2),Y(4),P(4),E(2),X(4),
                                                Z(2)
      COMMON/A/IP,T4,SF,XB
C...Temp. tray 4(channel 17) and bottom's flow rate
      (channel 23)
      DATA IMULT/17,23/
C... Initial guess for tray compositions
      DATA X/.08,.13,.18,.23/
C...Enthalpy of saturated liquid
      ENTL(X) = 1800. -2433. *X+1753.*X**2
```

```
C...Enthalpy of saturated vapor
    ENTV(X) =11440.-1990.*X
C...Initialised values of tray 4 temp., bottom's flow
    rate and steam flow rate
    T40=82.7371
    B0=.53*.53*10.
    SF0=3.234
C...Initial data
    ERINT=0
    XKC=0.9
    TI=30
    XB=.05
    XBSET=.005
    IFLAG=1
    ICOUNT=1
    IP=1
    TS1=60.
    TS=10
    EFFS=.459
C...Calculate tray pressures
    P1=1.35
    DP=.6
    P1=1.+P1/14.7
      DP=DP*50./(32.*12.)
    PB=P1
    DO 35I=1,4
```

```
 35  P(I)=P1-FLOAT(I)*DP/24.
     XBSET=XB
     QLT=83392
     SFSET=3.234
C...Maintain constant steam flow rate until steady state
     attained
     IOUT=.77*.77*10.*204.7
C...Steam flow rate controller setpoint(channel 2)
201    CALL AOUT(2,IOUT,IER)
     CALL WAIT(30,2,IERR)
     IF(IP.EQ.1) GO TO 201
     ITS=TS
C...Scan analog inputs
31   CALL AIRDW(2,IMULT,IN,ISTAT)
     VAR(1)=10.*IN(1)/102.4+11.5
     VAR(2)=IN(2)/102.4
     IF(IFLAG.EQ.1) GO TO 41
C...Digital filtering of input signals
     A1=(2.*TS1-TS)/(2.*TS1-TS)
     A2=TS/(2.*TS1+TS)
     DO 32 I=1,2
32   E(I)=A1*E(I)+A2*(VAR(I)+Z(I))
     GO TO 51
41   DO 42 I=1,2
42   E(I)=VAR(I)
     IFLAG=2
```

```
51  DO 52 I=1,2
52  Z(I)=VAR(I)
    ICOUNT=ICOUNT+1
    IF(ICOUNT.NE.60) GO TO 61
C...Steady state values of tray 4 temp., bottom's flow
    rate and steam flow rate
    T41=E(1)
    B1=E(2)
61  CONTINUE
C...Composition setpoint change given after ten minutes
    IF(ICOUNT.LT.61) GO TO 15
C...Calculate actual values of tray 4 temp., bottom's
    flow rate and steam flow rate to be used for estima-
    tor calculations
    T4=T40+(E(1)-T41)
    BGPM=BO+(E(2)-B1)
    BGPM=SQRT(BGPM/10.)
    SF1=SFO+(SF-3.234)
C...Calculate value of XB for which the difference be-
    tween calculated and recorded value of tray 4 temp.
    is less than error criterion
    V = T4
C...Error criterion
    ERR=.0006
    DB=.001
    CPM=-1.
    CPL=-1.
```

```
      LOOP=1
      CALL TICKS(INT1)
20    CALL EQUIL(XB,YB,TB,PB)
      B=BGPM*RO(XB,TB)*3785.
C...Calculate reboiler heat input
      QB=SF1*13538.*60./3.234-0.33*QLT
C...Calculate tray heat loss
      QL1=QLT*.666/24./B
      DQB=QB/B-ENTL(XB)
C...Calculate reboiler vapor composition
      YB-XB+EFFS*(YB-XB)
C...Calculate X(1) using value of YB by trial and error
      DX=.002
      DXBGM=-1.
      DXBGP=-1.
1     YB1=X(1)+(ENTV(YB)-ENTL(X(1)))*(X(1)-XB)/(DQB+ENTL
                                             (X(1)))
      IF (ABS(YB1-YB).LT..000001) GO TO 2
      CALL ADJUST(YB1,YB,DXBGP,DXBGM,X(1),DX)
      GO TO 1
C...Calculate Y(1) using value of X(1)
2.    CALL EQUIL(X(1),YX,T,P(1))
      Y(1)=(1.-EFFS)*YB+EFFS*YX
C...Calculate tray 4 temperature
      DO 7 I=1,3
C...Calculate X(I+1) for a given value of Y(I) by trial
      and error
```

```
10     DX=.002
      CLAGM=-1.
      CLAGP=-1.
3     YY=X(I+1)+(ENTV(Y(I))-ENTL(X(I+1)))*(X(I+1)-XB)/
                              (DQB+ENTL(X(I+1))
     1-QL1*FLOAT(I))
      IF(ABS(Y(I)-YY).LT..000001) GO TO 4
      CALL ADJUST(YY,Y(I),CLAGM,CLAGP,X(I+1),DX)
      GO TO 3
C...Calculate Y(I+1) using Murphree tray efficiency
4     CALL EQUIL(X(I+1),YX,T,P(I+1))
      Y(I+1)=(1.-EFFS)*Y(I)+EFFS*YX
7     CONTINUE
      LOOP=LOOP+1
C...Compare recorded and calculated value of tray 4 temp.
      IF(ABS(T-V).LT.ERR) Go To 23
      IF(LOOP.GT.35) GO TO 23
C...Make another guess for bottom's composition
      CALL ADJUST(V,T,CPL,CPM,XB,DB)
      GO TO 20
23    ERROR=-(XBSET-XB)
      CALL TICKS(INT2)
C...Time required for estimator calculations
      ITIME=INT2-INT1
      TS=10.+FLOAT(ITIME)/60.
      IF(SF.GT.3.78.AND ERROR GT. 0) GO TO 15
```

```
      ERINT=ERINT+ERROR*TS*XKC/TI
      SF=SFSET+XKC*ERROR+ERINT
      IF(SF.GT.3.78) ERINT=0
      IF(SF.GT.3.78) SFSET=3.781
      IF(SF.GT.3.78) SF=3.781
      COUT=(SF/4.2)**2*10.
      IOUT=COUT*204.7
C...Steam flow rate controller setpoint(channel 2)
        CALL AOUT(2,IOUT,IER)
15    CALL WAIT(ITS,2,IER)
      GO TO 31
      END
```

```
      FUNCTION RO(X,T)
C...Calculates molar density(gmoles/cc) for given liquid
      composition temperature
      RO=1./(32.04*X/(.80999-.0009253*T-.00000041*T**2)
                                 +18.016*(1.-X)/1(100523-0002135
                                 *T+.00000255*T**2))
      RETURN
      END


      SUBROUTINE EQUIL(X1,Y1,T,P)
C...This subroutine calculates the equilibrium vapor
      composition and temperature for a given liquid compo-
      sition and total pressure
      X2=1.-X1
      LOOP=1
      GAM1=EXP(0.9*X2**2/(0.9*X1/0.48+X2)**2)
      GAM2=EXP(0.48*X1**2/(X1+0.48/0.9*X2)**2)
      T=64.7*X1+100.*X2
      T=T+273.15
1     CONTINUE
      P1=EXP(-4386.9/T+12.9848)
      P2=EXP(-4981.036/T+13.3486)
      ERR=P-GAM1*X1*P1-GAM2*X2*P2
      T1=T
      LOOP=LOOP+1
```

```
      IF(LOOP.GT.50) GO TO 4
      DER-GAM1*X1*P1* 4386.9/T**2 +GAM2*X2*P2* 4981.036/T**2
      DER=-DER
      T=T-ERR/DER
      IF(ABS(T1-T).LT..00001) GO TO 4
      GO TO 1
4     Y1=X1*P1*GAM1/P
      T=T-273.15
      RETURN
      END


      SUBROUTINE ADJUST(51.52,FLAGM,FLAGP,A,DA)
C...Makes a new guess for interval halving convergence
      method
      IF(S1-S2) 1,2,3
1     IF(FLAGM.LT.0) GO TO 4
      DA-DA/2
4     A=A+DA
      FLAGP=1
      GO TO 2
3     IF (FLAGP.LT.0) GO TO 5
      DA=DA/2
5     A=A-DA
      FLAGM=1
2     IF(A.LT.0.0005) A=0.0005
      RETURN
      END
```

NOMENCLATURE (EQUATIONS)

B	Bottom's flow rate (gmoles/min)
D	Distillate flow rate (gmoles/min)
EFFR	Murphree tray efficiency in the rectifying section
EFFS	Murphree tray efficiency in the stripping section
H	Enthalpy of saturated vapor (cal/gmole)
h	Enthalpy of saturated liquid (cal/gmole)
L	Liquid flow rate (gmoles/min)
NT	Total number of trays
N	Tray number
QB	Effective reboiler heat input (cal/min)
QC	Condenser heat load (cal/min)
QL	Tray heat loss (cal/min)
R	Reflux flow rate (gmoles/min)
SF	Steam flow rate (kg/min)
T	Tray temperatures ($^{\circ}$C)
V	Vapor flow rate (gmoles/min)
x	Liquid composition (mole fraction)
y	Vapor composition (mole fraction)

SYMBOLS

*	Equilibrium composition

SUBSCRIPTS

B	Bottom's
D	Distillate
n	Tray
NT	Top tray
NF	Feed tray

NOMENCLATURE (PROGRAM LISTINGS)

B	Bottom's flow rate
B1	Steady state recorded value of bottom's rate (RE1 estimator)
BGPM	Bottom's flow rate in gpm (for use in RE1 estimator)
BO	Initialized steady state value of bottom's rate (RE1 estimator)
EFFS	Murphree tray efficiency in the stipping section
ENTV	Enthalpy of saturated vapor
ENTL	Enthalpy of saturated liquid
PB	Column base pressure
P	Tray pressure
QB	Effective reboiler heat input
QLT	Total heat loss in the column plus reboiler
RO	Molar density
SF	Steam flow rate setpoint
SFSET	Steady state steam flow rate setpoint
SF1	Steam flow rate (for use in RE1 estimator)
SFO	Initialized value of steam flow rate (RE1 estimator)
TI	Reset time
T_4	Tray 4 temperature (for use in RE1 estimator)
T_{41}	Steady state value of tray 4 temperature (RE1 estimator)
T_{40}	Initialized value of tray 4 temperature (RE1 estimator)
TSET	Steady state values of tray temperatures (Brosilow's linear estimator)
TS1	First order lag in digital filter

TS	Sampling period
T	Tray temperature
XB	Bottom's product composition
XKC	Controller gain
XBSET	Bottom's product composition setpoint
X	Tray liquid composition
YX	Equilibrium vapor composition
Y	Tray vapor composition
YB	Reboiler vapor composition

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