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Title: DYNAMICS AND CONTROL OF A HEAT INTEGRATED DISTILLATION COLUMN WITH SIDE HEAT EXCHANGERS

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One of the alternative energy-saving methods in a conventional distillation process is the use of side (intermediate) reboiler and/or condenser for a portion of the overall heat load. A nonlinear differential equations model was developed to describe the dynamics of a typical binary distillation process with and without the side heat exchangers. Conventional column dynamics can be represented by 2x2 transfer matrices, whereas for a column with side heat exchangers the open-loop and closed-loop dynamics can be expressed in terms of 4x4 transfer matrices.

Analysis indicates that decoupling and feedforward control policies may be hard to implement, due to the increased dimensionality. However, simplifications obtained through the selective pairing of the control variables provide the familiar 2x2 matrix treatment. Classical control policy was extended to design different control strategies (feedback and feedback/feedforward)

for a column with side heat exchangers. Simulation studies reveal that the control response is better in the case of the modified column. When the side heat exchanger duties were used as feedforward variables with reflux and main boil-up rates as feedback variables, little improvement was observed as compared to the feedback control alone. On the other hand, use of side heat exchanger duties as feedback variables with reflux and main boil-up rates as feedforward variables resulted in unstable operation of the column.

Dynamics and Control of a Heat Integrated Distillation Column with Side Heat Exchangers

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1. INTRODUCTION

Distillation is the most commonly used separation process in the petroleum and chemical industries. It is the largest energy consumer among all the process units in the petrochemical plants, and it was reported (1) that 40-50% of the energy consumption in the petrochemical plants is taken by the distillation equipments. During the past few years many investigations have been made to improve the energy efficiency of the distillation process. Vapor compression, thermal coupling, multiple effect heat integration, and others have been suggested.

One of the alternative energy-saving methods is the use of side (intermediate) reboilers and/or condensers for a portion of the overall heat load. These heat exchangers remove heat at a higher temperature than the main condenser and provide heat at a lower temperature than the main reboiler. Thus there is a net increase in the thermodynamic efficiency of the column. In principle, it is possible to introduce the overall heat load throughout the stages below the feed and remove the necessary heat throughout the stages above the feed at the expense of additional stages for the same operation. But from an economic standpoint, when it is advantageous to add intermediate condensers and/or reboilers, only one of each would be sufficient. However, the effectiveness and the efficiency of the distillation operation cannot be achieved without a well-designed control system. An energy efficient distillation column should be designed in coordination with computer simulation, equipment design and distillation control.

Unfortunately, no published data about the dynamics and control of a distillation column using side heat exchangers is available in the literature. On the other hand, the optimum locations and duties of the side heat exchangers have been established. A comparative study on steady state simulations of a conventional distillation column and a distillation column with side heat exchangers was done by Mah (1) who reported that substantial reduction (about 50%) in steam and cooling water consumption could be realized in the latter case.

The objective of this thesis is to analyze the effects of the intermediate heat exchangers on the dynamics of a distillation column and to study some possible ways of incorporating these new features into the control strategies established by classical control. Two binary distillation columns, one a conventional column, and another with side heat exchangers were chosen for a comparative study. A rigorous nonlinear differential equation model was developed to describe the distillation process. The necessary transfer functions representing dynamic behavior of the distillation columns were obtained by simulating the model on computer. A classical control scheme was designed for the conventional column. Different control policies were investigated for the distillation column with side heat exchangers, and the corresponding control responses of both the columns were compared.

2. LITERATURE SURVEY

Distillation is the most important separation unit operation in the process industry. It is widely used to upgrade feed stocks, separate reaction intermediates, and purify products. In petroleum refineries, which are the largest energy consumers, crude distillation alone accounts for 22 to 51% of the total energy consumption (1).

In the conventional column, heat is supplied to the reboiler and removed from the condenser. Because of the temperature difference between the reboiler and the condenser, the separation of components is always accompanied by a degradation of energy, when we view it as a thermodynamic process. Conventional distillation is not particularly noted for its efficiency. Estimates as low as 1.9% have been reported for the thermodynamic efficiency of industrial distillation columns (2).

Although various alternatives in their design to economize heat consumption have been established--as summarized by Robinson and Gilliland (3), Benedict and Pigford (4), Pratt (5) and King (6), the applications of these models were not seriously considered until the energy crunch, when it became increasingly necessary to explore all the possible energy saving schemes in the design of new equipments. For example, Null (7) reported possible savings by using heat pump and recompression cycles and O'Brian (8) indicated the reduction of steam consumption by the use of double-effect columns. Furthermore, two other applications which are reported by Duckham and Fleming (9) show that use of a heat pump and an intermediate boiler in two different cases produced significant improvement in heat consumption. Use of an intermediate boiler and condenser was analyzed by Timmers (10), as an alternative to reduce the cost of distillation, and suggested a design criterion based on minimized column volume. Tyreus and Luyben (11) made extensive digital simulation studies of the dynamics and control of multiple heat integrated distillation columns (Propylene-propane and methanol-water). They reported that an auxiliary reboiler on the low pressure column and/or an auxiliary condenser on the high pressure column provide an improved flexibility on the operation of the columns.

Perhaps the most significant analysis of the importance of intermediate heat exchangers is due to Mah (1). He made a comparative study of steady state simulations using a conventional column and a distillation column with side heat exchangers on propylene-propane, ethylene-ethane, ethane-butane and two other systems, and reported that a substantial reduction (50-70%) in steam and cooling water consumption could be realized in the latter case.

In contrast to the modifications using multiple-effect integration or vapor compression, in which the internal vapor and liquid flows remain unaltered, in a distillation column using side heat exchangers the reflux and vaporization rates are deliberately manipulated to enhance the overall thermal efficiency. In this scheme, the liquid reflux rate increases as we proceed down the rectifying section, and the vapor flow rate increases as we proceed up the stripping section as a result of the heat exchangers between the two sections. Besides the obvious effect of reducing the reboiler and condenser duties, the introduction of secondary reflux and vaporization also modifies the operating lines, as shown in Figure 1. Of course, for a given total number of stages and total heat duty, the separation will be slightly lower in the distillation column using intermediate heat exchangers.

Furthermore, it is important to know the dynamics and control response of the distillation column with side heat exchangers for a stable operation of the column. Unfortunately, there is hardly any published data available in literature as far as the dynamics and control

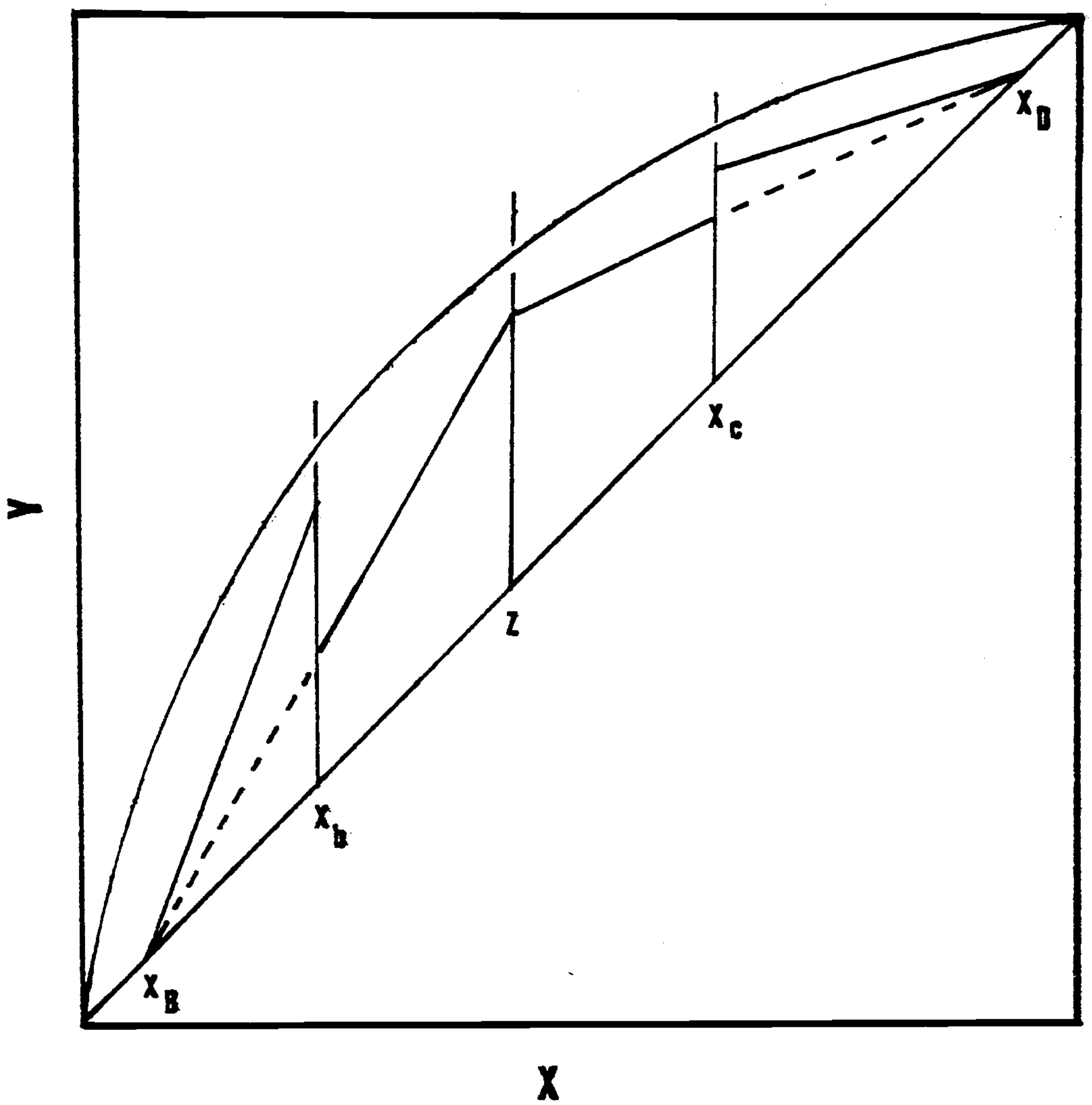

Figure 1. Operating lines for a binary distillation column with an intermediate condenser and a reboiler. The operating line for the conventional case is shown by dashed lines and for both cases the total heat loads are the same.

are considered. By initial analysis, one could expect a better (faster) dynamic response using the intermediate heat exchangers, due to the fact that the disturbance has to travel a lesser time before there is any change in liquid and/or vapor flow inside the column.

The main aspect of a distillation column operation is the regulatory control, where the objective is to maintain process variables (usually product compositions) at their prescribed set points in case of disturbances. Invariably, reflux rate and boil-up rates are used as control (manipulated) variables to control the top and bottom product compositions (controlled variables), using feedback control schemes. Distillation being a multivariable and multistage process, it becomes extremely difficult to control the product compositions because of the inherent interaction between the control loops. For example, changes in vapor boil-up to control the bottoms product composition also affect overhead composition. Likewise, changes in reflux flow to control distillate composition disturb bottom composition. Several discussions of interaction in distillation control and possible ways to overcome interaction have appeared in literature. Rijnsdorp (13) proposed a ratio control scheme between reflux and top vapor flow to reduce the interaction effects. Buckley (14) suggested a more practical scheme (due to its simplicity) of inserting two interaction compensators, much like feedforward controllers, to cancel out the effects of each manipulative variables on the composition at the opposite end of the column. Luyben (15) studied the design and performance of Buckley's simplified decouplers and an ideal decoupler for several binary distillation columns, and concluded that simplified decouplers offer almost the same performance as that of the ideal decoupler. Moreover, he found that in certain cases the ideal decoupling might lead to unstable operation of the distillation column. Wood and Barry (16) did a comparative study of the non-interacting control scheme using simplified decouplers as suggested by Luyben, and ratio control suggested by Rijnsdorp. They found marginal improvement in the case of ratio control over the other, and preferred the decoupler design as suggested by Luyben, due to its simplicity.

Shinskey (17, 18) discussed the advantages of using feedforward control of the distillation column, and reported that very little attention has been given to the use of feedforward control in the industrial columns. The need for feedforward control results from the fact that feedback control is based on an error, i.e., a deviation between set point and measurement. In processes such as distillation that are characterized by large-time-constants and dead times, disturbances in feed rate or composition have a pronounced long term effect on the operability of the column. Feedforward obviates this problem by predicting in advance the effect of measurable load disturbance on product compositions. The feedforward model, which relates the controlled variable to the disturbance variables, takes the necessary control action before the disturbance can manifest itself on a product quality deviation.

Luyben (19) suggested a design scheme of feedback/feedforward control of a binary distillation column, wherein feedforward control was applied to the control variables (reflux and/or vapor boil-up rate) with a feedback from some intermediate stage compositions. His analysis showed that holding intermediate stage compositions (due to feedback control) will not necessarily keep product compositions constant. Thus the feedforward controller, which conventionally changes manipulated variables, has the additional job of adjusting the feedback controller set points.

This basic idea of a feedback/feedforward control scheme could be extended to design a control scheme for a binary distillation column with intermediate heat exchangers, the difference being that we have two more manipulated variables, namely, the intermediate heat exchanger duties. The main problem in synthesizing a feedback/feedforward control in this case would be the increased dimensionality of the process matrices which are used in designing the control loop. One way of overcoming this problem would be by the selective pairing of the manipulated variables and treatment of the control loop synthesis, as in the case of a conventional column. For example, if it is decided to use reflux flow and main boil-up as the feedback control variables, then a feedforward scheme using intermediate heat exchanger duties as the control variables could be designed. In the same way, one could use intermediate heat exchanger duties as feedback control variables and the main boil-up and reflux rates as the feedforward control variables.

For a better design of a control scheme and control elements, it is extremely important to have a mathematical model which sufficiently describes the transient or dynamic behavior of a distillation column. Several authors (20, 21) have proposed steady state algorithms for distillation control, which are very easy to estimate as an approximate prediction of column operability, without going through the rigorous dynamic response of the column. Perhaps these correlations could be used for a quick testing of existing distillation column performance. But, Rosenbrock (22) and Harriot (23) stressed the importance of the dynamics for better control, and gave a critical review of different types of mathematical models representing the dynamic behavior of a distillation column. Distillation being a complex, interacting, nonlinear multivariable system, it is extremely difficult to come up with a single mathematical model (representing both energy and material balance) and yet easy to simulate its performance. Most of these models are either too complex or take too much of computer time to simulate the process. These models involve either stage by stage or simultaneous solution of several differential and algebraic equations. Many assumptions and simplifications were suggested to reduce this complexity of the problem. Comparison and justification of these simplified models is discussed by McCune and Gallier (24). Perhaps the model proposed by Gould (25) is much simpler to simulate, yet maintains the important factors related to the dynamic behavior of a distillation column. The model is based on material balance only, and if needed, the heat effects (losses) could be easily incorporated in terms of either vaporization or condensation on each stage.

3. THEORY

Dynamic behavior of a typical distillation column can be described by two types of models. One is a linear model which is used for control law computations. This model was not used, due to certain difficulties encountered as explained in Appendix A. The second model is a rigorous nonlinear differential equation model, which considers the major factors affecting the column performance. All the design and simulation work in this thesis was based on this dynamic nonlinear model.

3.1 Dynamic Model

A mathematical model for the dynamic behavior of a plate column of a binary distillation process can be represented by (see Fig. 2), a mass balance on the light component in the liquid phase for the rth tray

$$\frac{d(H_r x_r)}{dt} = V_{r-1} y_{r-1} - V_r' y_r' + L_{r+1} x_{r+1} - L_r x_r + F_r z_r - J_r x_r \qquad (1)$$

a mass balance on the light component in the vapor phase

$$\frac{d(h_r y_r)}{dt} = V_r' y_r' - V_r y_r + F_r' z_r' - J_r' y_r \qquad (2)$$

an overall mass balance on the liquid phase

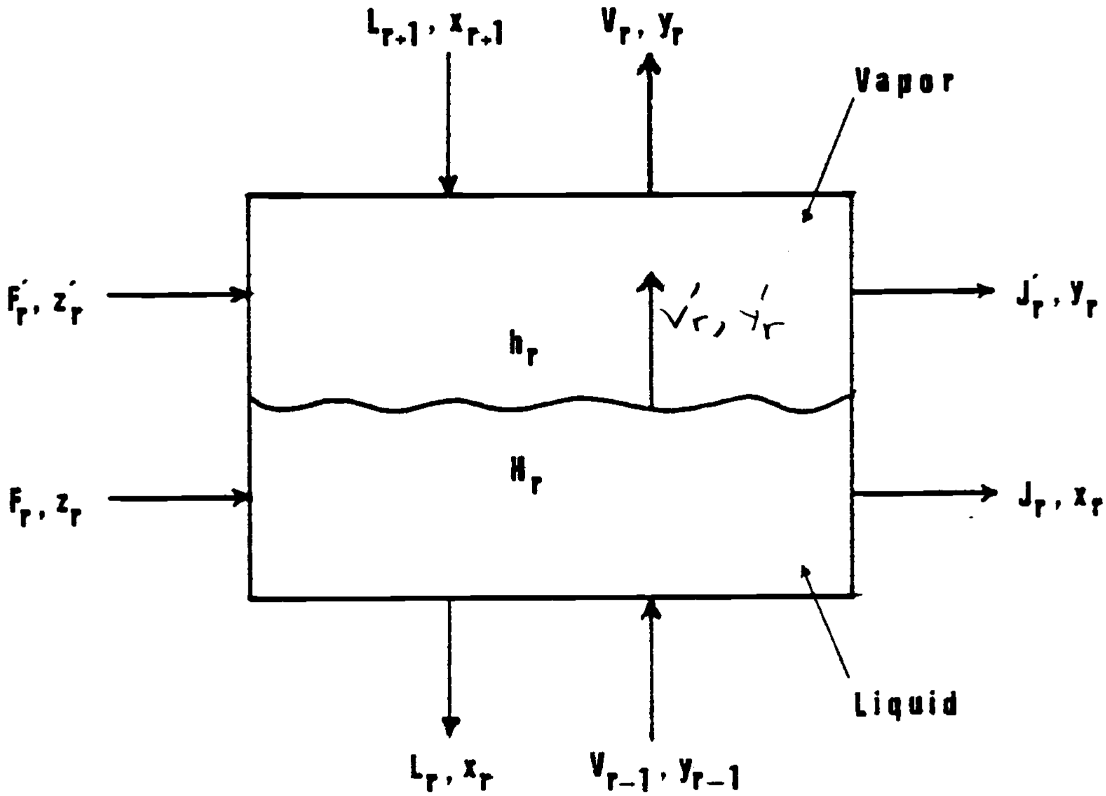

Figure 2. rth stage of a binary distillation column.

$$\frac{dH_r}{dt} = L_{r+1} - L_r + F_r - J_r + V_{r-1} - V_r' \tag{3}$$

an overall mass balance on the vapor phase

$$\frac{dh_r}{dt} = V_r' - V_r + F_r' - J_r' \tag{4}$$

and the vapor-liquid equilibrium is given by

$$y_r^* = f(x_r P_r) \tag{5}$$

where p_r is the pressure above the plate. If the vapor leaving the liquid on the rth tray is in equilibrium with the liquid, then, $y_r^* = y_r'$. However, if the plate is not ideal, then one usually introduces the plate efficiency in addition to equilibrium curve, namely,

$$E_r = \frac{y_r' - y_{r-1}}{y_r^* - y_{r-1}}. \tag{6}$$

The liquid flow L_r is generally a nonlinear function of the hold-up H_r on the tray and can be represented by

$$L_r = h(H_r). \tag{7}$$

If equilibrium is assumed and if the latent heat of vaporization is constant, and if there is no vapor hold-up in the liquid, then

$$V_{r-1} = V_r'. \tag{8}$$

The vapor hold-up above the plate is a function of pressure above the plate, i.e.,

$$h_r = h(p_r). \tag{9}$$

The above equations 1 through 9 should suffice to determine the behavior of a binary distillation column with no heat effects. However, this formulation, although useful for direct simulation, is generally too complicated and can be simplified when actual operating conditions are considered.

The first simplification is to neglect vapor phase hold-up h_r. Usually product is withdrawn in the liquid phase so that $J_r^{'} = 0$. In addition, if all the feed enters at or below the bubble point there is no vapor feed so that $F_r^{'} = 0$. Under these conditions the vapor rate, $V_r^{'}$, is continuous throughout the system, except at the reboiler and at condenser, say, V. Then equations 1 and 3 become

$$\frac{d(H_r x_r)}{dt} = V(y_{r-1} - y_r) + L_{r+1}x_{r+1} - (L_r + J_r)x_r + F_r z_r \tag{10}$$

$$\frac{dH_r}{dt} = L_{r+1} - L_r + F_r - J_r. \tag{11}$$

For the reboiler (which is numbered as 0th tray), the vapor is discontinuous and is controlled by the energy input to the reboiler. Similarly, for the condenser (which is numbered as (N+1)th tray), vapor flow is discontinuous if there is total condensation. The behavior of reboiler and condenser can be represented by

$$\frac{d(H_0 x_0)}{dt} = -Vy_0 + L_1 x_1 - Bx_B \tag{12}$$

$$\frac{dH_0}{dt} = L_1 - B - V \tag{13}$$

and

$$\frac{d(H_{N+1} x_D)}{dt} = Vy_N - (L_{N+1} + D)\ x_D \tag{14}$$

$$\frac{dH_{N+1}}{dt} = V - L_{N+1} - D. \tag{15}$$

The feed tray can be represented by

$$\frac{d(H_f x_f)}{dt} = V(y_{f-1} - y_f) + L_{f+1} x_{f+1} - L_f x_f + Fz_f \tag{16}$$

$$\frac{dH_f}{dt} = L_{f+1} - L_f + F. \tag{17}$$

Equations 10 through 17 describe the behavior of a distillation process with negligible hold-up in the vapor phase, and continuous vapor flow. They account for the possibility of variations of liquid hold-up during a flow transient. Although the liquid transient plays an important role, the relative speeds of the composition and flow transients are such that, one can ignore the flow transient to obtain a simpler but more manageable representation of the system.

When liquid hold-up is assumed constant, the liquid flow through each half of the system is continuous. Discontinuity in liquid flow occurs at the condenser, reboiler and feed tray. If L_u is the liquid rate in the upper half of the column and L_l is the rate in the lower half, equation 10 becomes

$$H\frac{dx_r}{dt} = V(y_{r-1}-y_r) + L_{l/u}(x_{r+1}-x_r). \qquad (18)$$

The reboiler equation becomes

$$H_0\frac{dx_B}{dt} = -Vy_0 + L_1x_1 - B\,x_B \qquad (19)$$

$$L_1 = B + V.$$

The condenser equation becomes

$$H_{N+1}\frac{dx_D}{dt} = Vy_N - (L_u+D)\,x_D \qquad (20)$$

$$V = L_u + D.$$

The feed tray equation becomes

$$H\,\frac{dx_f}{dt} = V(y_{f-1}-y_f) + L_ux_{f+1} - L_1x_f + Fz_f \qquad (21)$$

$$L_1 = F + L_u.$$

Equations 18 through 21 serve as a simplified version of a distillation column under the assumption that the vapor hold-up is negligible, liquid hold-up is constant and equilibrium boiling with constant latent heat. This approximate representation was used in evaluating the transfer functions in designing of the control schemes, and in the simulation work (Figs. 3 and 4).

3.2 Classical Control

Classical control refers to the product compositions control of a conventional binary distillation column, where, x_D and x_B are the controlled variables, L and V are the manipulated (control) variables and f and z are the measurable disturbances. Then, the dynamics of the column can be represented in Laplace domain as

$$\begin{pmatrix} x_D \\ x_B \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} L \\ V \end{pmatrix} + \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} f \\ z \end{pmatrix} \tag{22}$$

or $\quad x = Mu + Pw$

For feed-back control policy, we have

$$u = B\,(x^s - x) \quad \Leftarrow \text{ P mode (no ID)} \tag{23}$$

which gives the closed loop control as

$$x = MB\,(x^s - x) + Pw \tag{24}$$

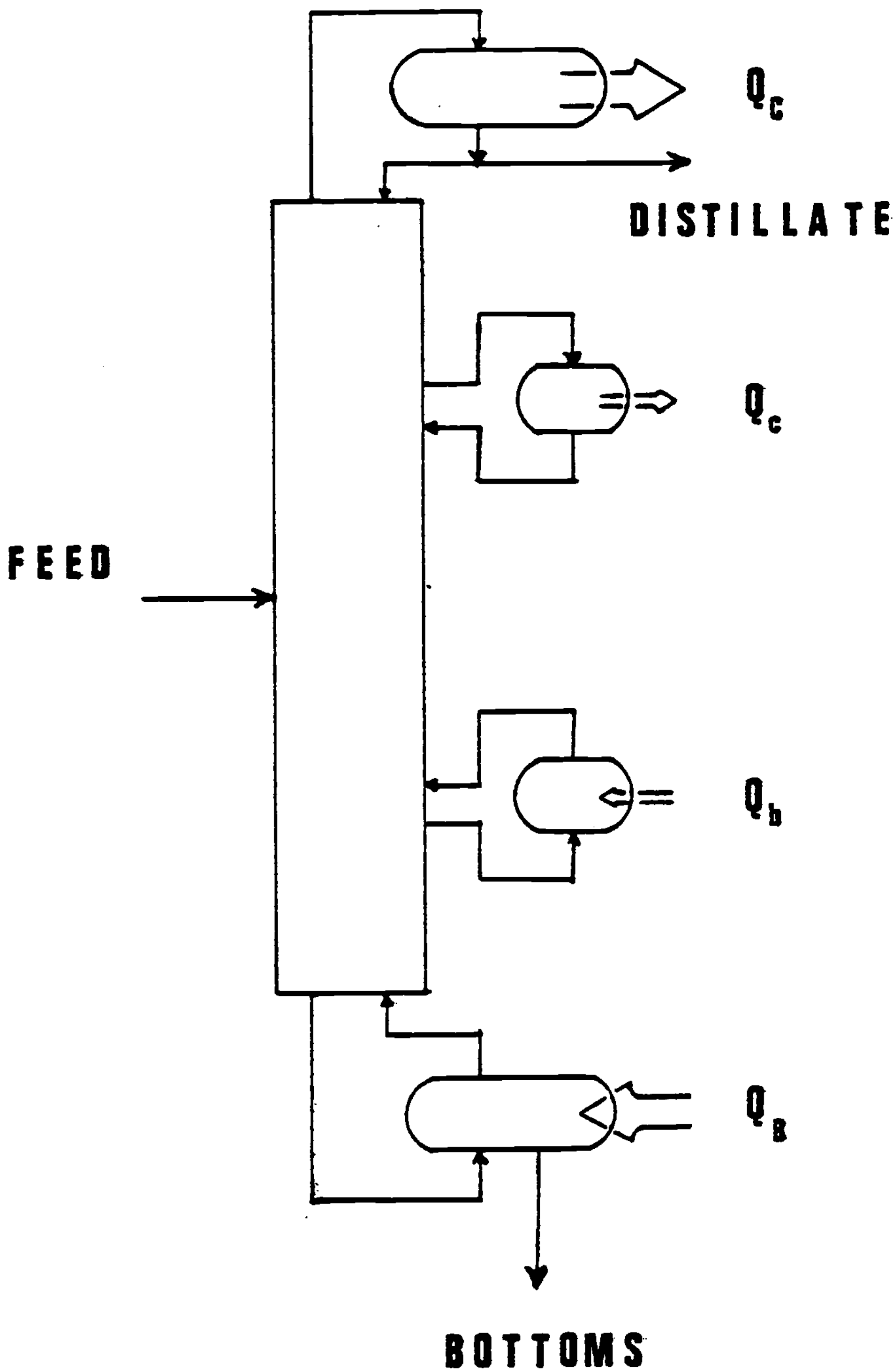

Figure 3. Distillation column with a side condenser and a reboiler.

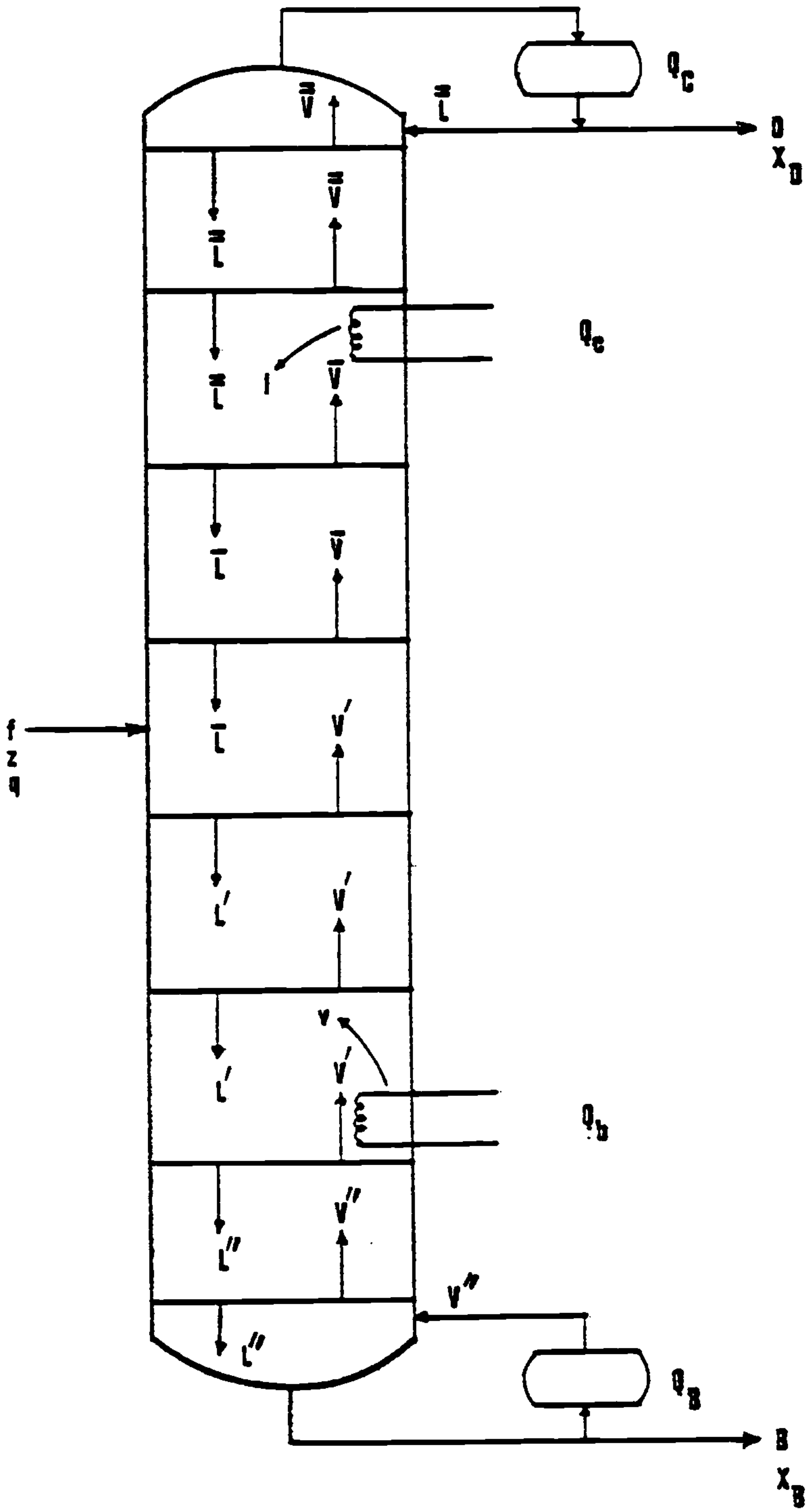

Figure 4. Internal flows in a typical distillation column with side heat exchangers.

where B is the diagonal matrix. To eliminate the interaction between the control loops, decoupling elements can be added. Then Equation 24 becomes

$$x = MDB\,(x^s - x) + Pw \tag{25}$$

or
$$x = (I+MDB)^{-1}\,MDB\,x^s + (I+MDB)^{-1}\,Pw \tag{26}$$

where D is the decoupling matrix.

For ideal decoupling, which means the response of each loop (with both on automatic control) should be the same as the response one would get if the other loop is on manual (thus fixing the other manipulated variable), we require $(I+MDB)^{-1}$ MDB to be diagonal. However, this may not be always realizable or it may cause closed loop instability (15). Instead, simple interaction compensators (simplified decouplers) may be as effective and more dependable (14, 15). For this case, we only require MD to be diagonal, where

$$D = \begin{pmatrix} 1 & D_{12} \\ D_{21} & 1 \end{pmatrix} . \tag{27}$$

With this simplified approach, the decoupling conditions are achieved when

$$D_{12} = -M_{12}/M_{11} \quad \text{and} \quad D_{21} = -M_{21}/M_{22}.$$

This control policy can be represented by the block diagram as shown in Fig. 5.

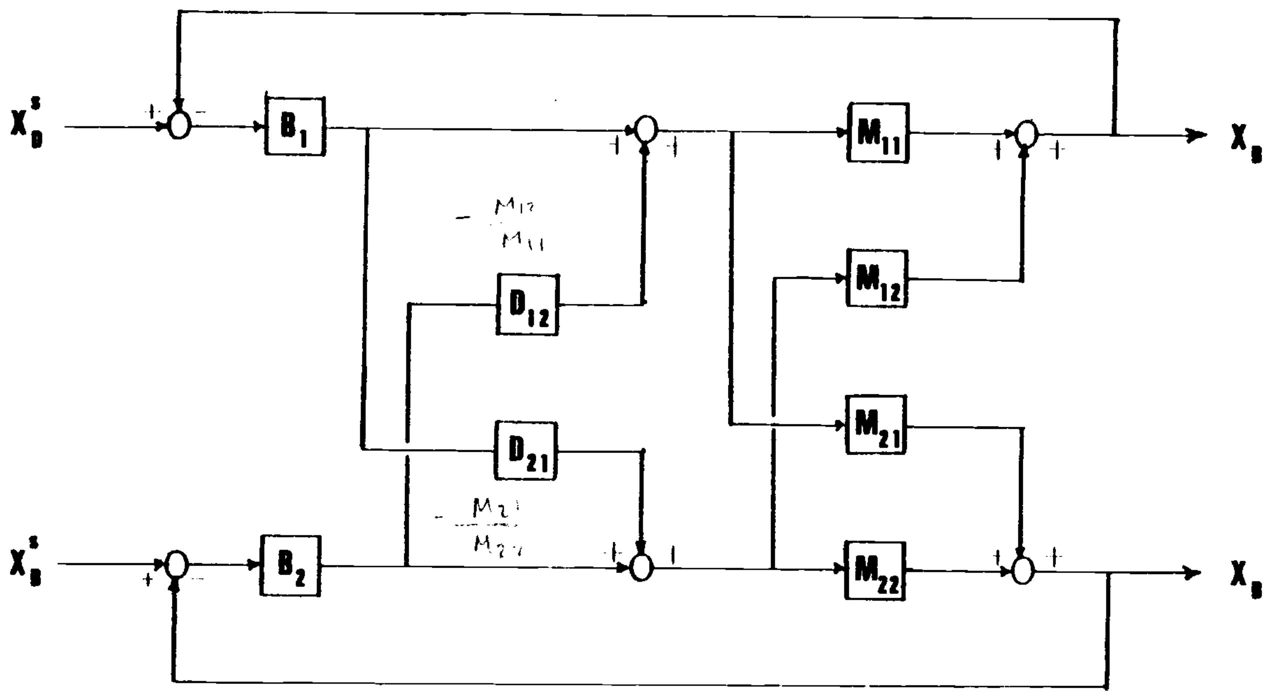

Figure 5. Block diagram representing classical control scheme.

Feedforward control can be added to the system if F can be designed such that

$$u = DB(x^s - x) + Fw. \tag{28}$$

The resulting closed loop equation

$$x = MDB(x^s - x) + (MF+P)w \tag{29}$$

$M^{-1}P$

indicates that the feedforward design requirement is

$$F = -M^{-1}P \tag{30}$$

Of course, the success of the feedforward design depends upon the realizability of M^{-1}.

3.3 Extension to the Modified Column

Luyben (19) suggested the use of intermediate stage compositions as feedback and reflux and boil-up rates as the feedforward variables, for a better control of the product compositions in a conventional column. This idea was used to extend the classical control policies to the heat integrated distillation column with side heat exchangers. However, the dimensionality of the problem is increased from 2x2 to 4x4. A typical distillation column with side heat exchangers is shown in Fig. 3. Here, the controlled variables are

$$X = (x_D \; x_B \; x_c \; x_b)^T$$

the manipulated variables are

$$U = (L \; V \; \ell \; v)^T$$

and the measurable disturbances are

$$w = (f \quad z).$$

Then, the dynamics of the column can be represented in Laplace domain as

$$\begin{pmatrix} x_D \\ x_B \\ x_c \\ x_b \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{pmatrix} \begin{pmatrix} L \\ V \\ \ell \\ v \end{pmatrix} + \begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \\ P_{31} & P_{32} \\ P_{41} & P_{42} \end{pmatrix} \begin{pmatrix} f \\ z \end{pmatrix}$$

or $$X = \tilde{M}u + \tilde{P}w. \tag{31}$$

For a feedback decoupling control, Equation 31 becomes

$$X = \tilde{M}\tilde{D}\tilde{B}\;(x^s - x) + \tilde{P}w \tag{32}$$

where B is the diagonal matrix and D is the decoupling matrix and both B & D are 4x4 matrices.

The higher dimensional matrices which are difficult to handle can be reduced to the familiar 2x2 matrices as in the classical control schemes. Then Equations 31 and 32 reduce to

$$\begin{pmatrix} x_I \\ x_{II} \end{pmatrix} = \begin{pmatrix} \bar{M}_I & \bar{M}_{II} \\ \bar{\bar{M}}_I & \bar{\bar{M}}_{II} \end{pmatrix} \begin{pmatrix} U_I \\ U_{II} \end{pmatrix} + \begin{pmatrix} P_I \\ P_{II} \end{pmatrix} w \tag{33}$$

and

$$\begin{pmatrix} x_I \\ x_{II} \end{pmatrix} = \begin{pmatrix} \bar{M}_I & \bar{M}_{II} \\ \bar{\bar{M}}_I & \bar{\bar{M}}_{II} \end{pmatrix} \begin{pmatrix} \bar{D}_I & \bar{D}_{II} \\ \bar{\bar{D}}_I & \bar{\bar{D}}_{II} \end{pmatrix} \begin{pmatrix} B_I & 0 \\ 0 & B_{II} \end{pmatrix} \begin{pmatrix} x_I^s - x_I \\ x_{II}^s - x_{II} \end{pmatrix} + \begin{pmatrix} P_I \\ P_{II} \end{pmatrix} w$$

or $$x = \tilde{M}\tilde{D}\tilde{B}(x^s - x) + \tilde{P}\,w \tag{34}$$

The 2x2 matrices $\bar{M}_I$ and P_I correspond closely, but not identical to their counterparts M and P, of the conventional column. From Equation 34, it can be concluded that the decoupler design requirement is

$$\tilde{M}\tilde{D} = \begin{pmatrix} \bar{M}_I\bar{D}_I + \bar{M}_{II}\bar{\bar{D}}_I & \bar{M}_I\bar{D}_{II} + \bar{M}_{II}\bar{\bar{D}}_{II} \\ \bar{\bar{M}}_I\bar{D}_I + \bar{\bar{M}}_{II}\bar{\bar{D}}_I & \bar{\bar{M}}_I\bar{D}_{II} + \bar{\bar{M}}_{II}\bar{\bar{D}}_{II} \end{pmatrix} \tag{35}$$

to be diagonal. Here, $\tilde{D}$ is the 4x4 decoupling matrix with 1's in the diagonal, similar to D defined in Equation 6. Therefore, the design of interaction compensators require the solution of the remaining 12 D_{ij}'s compared to only 2 of such elements in the conventional case.

The corresponding block diagram for the feedback closed loop control system is given in Fig. 6.

Incorporating the feedforward control, we get

$$\begin{pmatrix} U_I \\ \\ U_{II} \end{pmatrix} = \tilde{D}\tilde{B}\left[\begin{pmatrix} G_I \\ \\ G_{II} \end{pmatrix} w - \begin{pmatrix} x_I \\ \\ x_{II} \end{pmatrix}\right] + \begin{pmatrix} F_I \\ \\ F_{II} \end{pmatrix} w \tag{36}$$

where G_I and G_{II} are set point tracking matrices. Set point tracking matrices are needed to adjust the set points of feedback control of the intermediate exchanger duties, since controlling the intermediate stage compositions does not necessarily keep the product compositions constant. For the binary distillation control problem, the main job is to keep the product compositions constant; i.e., x_D and x_B are fixed. Hence, $G_I = 0$. Whereas, x_c^s and x_b^s are not necessarily constant to keep x_D and x_B at their prescribed levels. G_{II} a 2x2 matrix will adjust set points x_c^s and x_b^s as w changes. Therefore, equation 36 reduces to

$$\begin{pmatrix} U_I \\ \\ U_{II} \end{pmatrix} = \tilde{D}\tilde{B}\left[\begin{pmatrix} 0 \\ \\ G_{II} \end{pmatrix} w + \begin{pmatrix} x_I^s - x_I \\ \\ 0 \quad -x_{II} \end{pmatrix}\right] + \begin{pmatrix} F_I \\ \\ F_{II} \end{pmatrix} w. \tag{37}$$

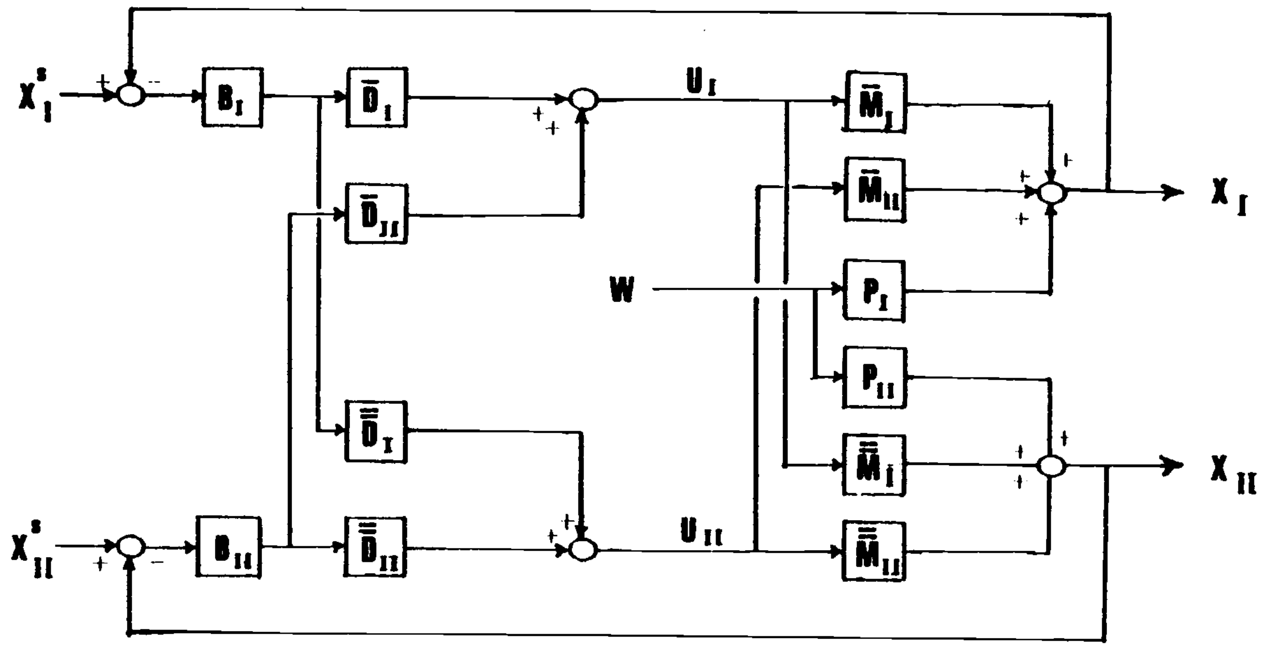

Figure 6. Block diagram representing feedback control of distillation column with side heat exchangers.

Considering only the disturbance effects on the controlled variables

$$\begin{pmatrix} x_I \\ x_{II} \end{pmatrix} = \left[\begin{pmatrix} \bar{M}_I & \bar{M}_{II} \\ \bar{\bar{M}}_I & \bar{\bar{M}}_{II} \end{pmatrix} \begin{pmatrix} F_I \\ F_{II} \end{pmatrix} + \begin{pmatrix} P_I \\ P_{II} \end{pmatrix} \right] w \tag{38}$$

the feedforward design conditions can be established. Therefore

$$\bar{M}_I F_I + \bar{M}_{II} F_{II} + P_I = 0 \tag{39}$$

and $\bar{\bar{M}}_I F_I + \bar{\bar{M}}_{II} F_{II} + P_{II} = G_{II}$. (40)

The variables in the above equations are F_I, F_{II} and G_{II}; one more than the number of matrix equations. Thus, we have the option of arbitrarily selecting either one of the feedforward matrices F_I or F_{II} or the set point tracking matrix G_{II}. For convenience, let us set $G_{II} = 0$, which then fixes x_c and x_b at the steady state levels. Now the solution for the feedforward matrix becomes

$$\begin{pmatrix} F_I \\ F_{II} \end{pmatrix} = -\begin{pmatrix} \bar{M}_I & \bar{M}_{II} \\ \bar{\bar{M}}_I & \bar{\bar{M}}_{II} \end{pmatrix}^{-1} \begin{pmatrix} P_I \\ P_{II} \end{pmatrix} \tag{41}$$

provided the indicated inverse exists. On the other hand, if we set $F_I = 0$, the required design conditions are

$$\bar{M}_{II}F_{II} + P_I = 0$$

$$\text{or} \quad F_{II} = -\bar{M}_{II}^{-1}P_I \tag{42}$$

$$\text{and} \quad \bar{\bar{M}}_{II}F_{II} + P_{II} = G_{II}$$

$$\text{or} \quad G_{II} = P_{II} - \bar{\bar{M}}_{II}\bar{M}_{II}^{-1}\, P_I \tag{43}$$

and if we set $F_{II} = 0$, we need

$$\bar{M}_I F_I + P_I = 0$$

$$\text{or} \quad F_I = -\bar{M}_I^{-1}\, P_I \tag{44}$$

$$\text{and} \quad \bar{\bar{M}}_I F_I + P_{II} = G_{II}$$

$$\text{or} \quad G_{II} = P_{II} - \bar{\bar{M}}_I \bar{M}_I^{-1} P_I \tag{45}$$

Again, the necessary matrix inverses must be realizable. Fig. 7 shows the block diagram representation of the 4x4 control system.

3.4 A Simplified Approach (Problem Identification)

As we can see from Equations 36 through 45, the decoupling and feedforward control design for the modified distillation column require the solution of higher order equations as compared to the conventional case, and thus have higher chances of not being realizable. However, we can relax some of the design and feedforward requirements, while maintaining most of the advantages of intermediate heat exchangers. The simplifications are obtained by applying feedback control through selective pairing of either x_I, U_I or x_{II}, U_{II} pair and feedforward through the other.

Consider the feedback through x_I, U_I pair. For this we get the following equation. (See Fig. 7.)

$$B_{II} = \bar{D}_{II} = \bar{\bar{D}}_I = \bar{\bar{D}}_{II} = F_I = G_{II} = 0 \tag{46}$$

The decoupling requirements reduce to having only $M_I D_I$ to be diagonal, which is identical in size to that of the conventional case. The feedforward controller design is also simplified to

$$\bar{M}_{II} F_{II} + P_I = 0$$

$$\text{or} \quad F_{II} = -\bar{M}_{II}^{-1} P_I. \tag{47}$$

On the other hand, for feedback through x_{II}, U_{II}, we get, (again, see Fig. 7.)

$$B_I = \bar{D}_I = \bar{D}_{II} = \bar{\bar{D}}_{II} = F_{II} = 0 \tag{48}$$

with decoupling requirements as $\bar{M}_{II}\bar{\bar{D}}_{II}$ to be diagonal. For feedforward control, the design matrix becomes

$$\bar{M} F_I + P_I = 0$$

$$\text{or} \quad F_I = -\bar{M}_I^{-1} P_I \tag{49}$$

$$\text{and} \quad G_{II} = P_{II} - \bar{\bar{M}}_I \bar{M}_I^{-1} P_I \tag{50}$$

The closed loop block diagrams for these alternatives

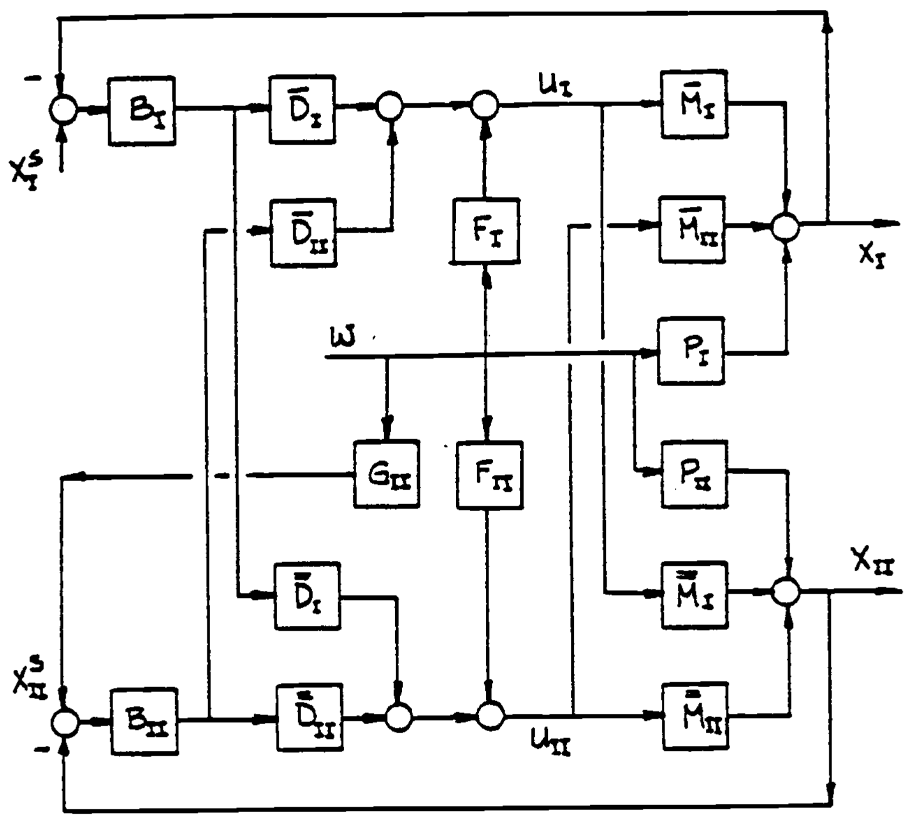

Figure 7. Block diagram representing feedback/ feedforward control of distillation column with side heat exchangers.

are given in Fig. 8 and Fig. 9.

These two control schemes were used to study the product compositions control response of a typical binary distillation column with side heat exchangers.

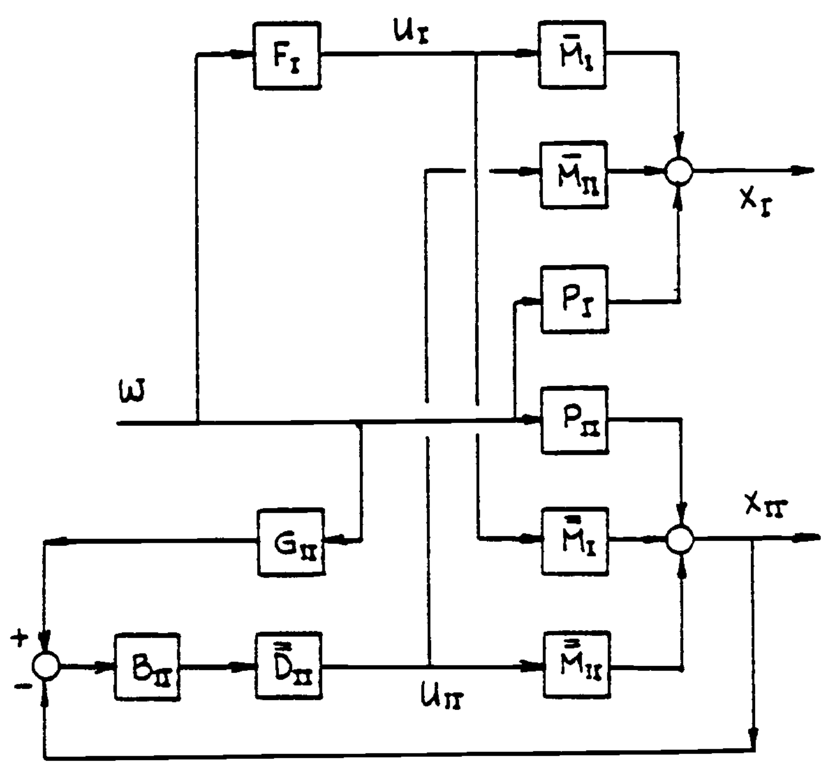

Figure 8. Modified column selective feedback and feedforward control scheme, case I.

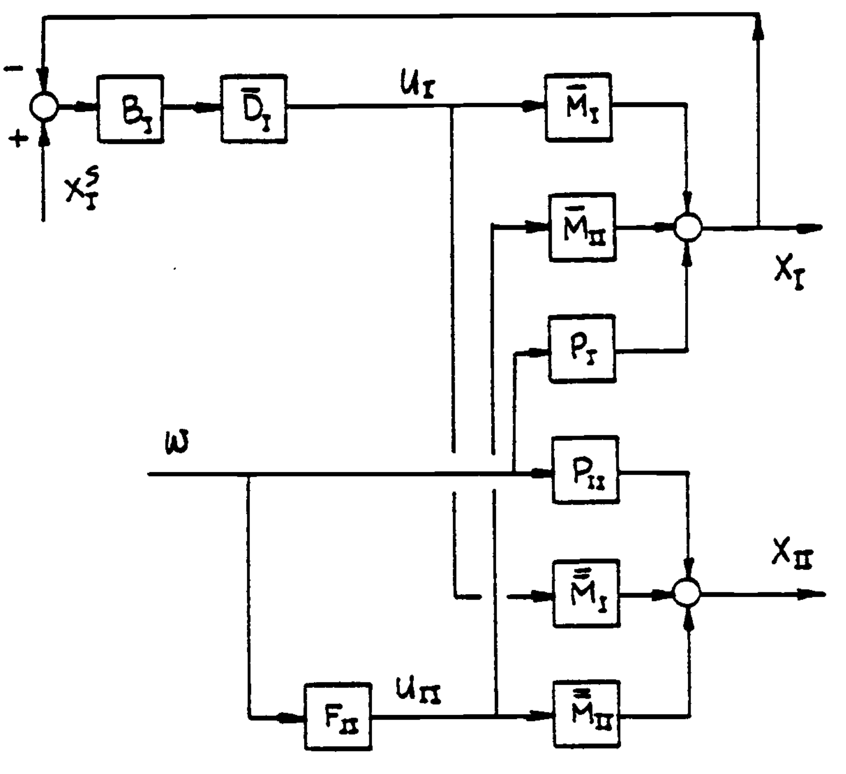

Figure 9. Modified column selective feedback/ feedforward control scheme, case II.

4.0 DESIGN CONSIDERATIONS

A typical binary separation system (relative volatility, α =2.0) was chosen, to design the number of stages required for a given separation (x_D=0.95 and x_B=0.05) using Smoker's equation (21). The optimum locations and heat duties of the intermediate heat exchangers were decided as suggested by Kayihan (12). A nonlinear differential equations model was developed and used as the basis for simulation to find the necessary transfer functions. A general form

$$g(s) = \frac{K_p(T_3s+1)\ e^{-\theta s}}{(T_1s+1)(T_2s+1)}$$

was used for each one of the transfer matrix elements. Open loop (steady state) gain, K_p, and time delay term, θ, are calculated from step response tests. The other parameters, T_1, T_2 and T_3 are screened and the significant ones are identified through a time domain least-square-fit analysis of column response to positive and negative pulses (a step change in series).

With $\alpha = 2.0$

$z = 0.5$

$x_D = 0.95$

$x_B = 0.05$

the minimum reflux ratio R_m, is given by

$$R_m = \frac{[x_D - z/(1+(\alpha-1)z)]}{[\alpha z/(1+(\alpha-1)z)-z]}$$

$$= 1.7.$$

It is a normal practice to use an actual reflux ratio of 1.1 to 1.5 times the minimum reflux ratio (9, 15), therefore, the actual reflux ratio is

$$R = 1.2x1.7 = 2.04.$$

The minimum number of ideal stages N_m, is given by

$$N_m = \frac{\ell n(\frac{x_D}{1-x_D})\ (\frac{x_B}{1-x_B})}{\ell n\ 2}$$

$$= 8.4959$$

and the actual number of ideal stages, N, is then calculated as

$$\frac{N-N_m}{N+1} = 0.75\left[1-\left(\frac{R-R_m}{R+1}\right)^{0.5668}\right]$$

$$= 0.5332.$$

which gives N = 19.35. Therefore, the total number of ideal stages can be approximately taken as 20.

The optimum locations and heat duties of the intermediate heat exchangers are given by

$$x_c = z^{\frac{1}{2}}$$

$$= 0.7071$$

$$x_b = 1 - (1-z)^{\frac{1}{2}}$$

$$= 0.2929$$

$$\frac{q_c}{Q_C+q_c} = 1 - z/x_c$$

$$= 0.3515$$

$$\frac{q_b}{Q_B+q_b} = 1 - (1-z)/(1-x_b)$$

$$= 0.3515$$

The exact locations of the intermediate heat exchangers are fixed at the stages, where the stage compositions are closest to the above compositions. As for the heat duties, total amount of heat load is kept constant for both conventional and modified columns as a basis for comparison of the column performances. Of course, this will result in slightly lower separation in the case of the modified column.

Finally, the feed rate, individual stage hold-ups as well as the reboiler stage hold-up, are specified and the top and bottom product rates are calculated by steady state material balance. These specifications of the conventional and modified columns are summarized in Table 1. Using these column characteristics, the nonlinear differential equations model is simulated using DVERK subroutine from the IMSL package to get the steady state compositions of each stage, and are listed in Table 2. These steady state conditions were used as the basis for all further calculations and simulation runs for the control response of the distillation columns.

4.1 Steady State Gains

Steady state gains, which are also referred to as process gains, show the extent of changes in products/ stage compositions when the distillation column is changed from one steady state to another, by changing control or disturbance variables. These can be determined either by taking partial derivatives of the particular composition with respect to the variable under consideration, or by numerical analysis technique (26). The latter technique, (which was also adopted in this thesis), involves rigorous solution of nonlinear differential equations. For example, to get the steady state gain of x_D with respect to change in feed rate, the feed rate is changed first by 10% (a positive step change) from its steady state value, keeping all the other

Table 1. COLUMN CHARACTERISTICS

	Conventional	Modified
α	2	2
N_T	20	20
N_F	11	11
N_{IB}		6
N_{IC}		16
f	100	100
z	0.5	0.5
x_D	0.9551	0.9459
x_B	0.0454	0.0538
x_b		0.2731
x_c		0.7237
H_{stage}	10	10
H_{boiler}	100	100

Table 2. STEADY STATE STAGE COMPOSITIONS

Stage	Conventional column	Modified column
1 (x_B)	0.0454	0.0538
2	0.0766	0.0876
3	0.1183	0.1289
4	0.1705	0.1760
5	0.2304	0.2258
6 (x_b)	0.2930	0.2741
7	0.3523	0.3371
8	0.4032	0.3928
9	0.4436	0.4378
10	0.4737	0.4716
11 (feed)	0.4949	0.4956
12	0.5186	0.5239
13	0.5497	0.5609
14	0.5891	0.6072
15	0.6368	0.6622
16 (x_c)	0.6913	0.7237
17	0.7501	0.7602
18	0.8093	0.8023
19	0.8649	0.8487
20	0.9141	0.8974
x_D	0.9551	0.9459

control and disturbance variables at their respective steady state values. The column was simulated to its new steady state and the change in x_D from its old steady state is noted. Then, the column is again simulated to its new steady state, by giving a similar 10% negative step change in feed rate from its original steady state. The change in x_D from its old steady state was also noted. The average of the above two changes per unit change in feed rate is the steady state gain of x_D with respect to the feed rate. The same process was repeated to evaluate process gains of x_D and x_B with respect to all the control and disturbance variables. The steady state gains for the conventional column are tabulated in Table 3. For the modified column, the process gains were evaluated for the controlled variables x_D, x_B, x_c and x_b, with respect to the control and disturbance variables feed rate, feed composition, main boil-up rate, reflux rate, and intermediate heat exchanger duties. These steady state gains are tabulated in Table 4. A sample computer output for steady state gain calculations is given in Appendix B.

4.2 Dynamic Response

Dynamic behavior of a distillation column was approximated by a set of transfer functions, which

Table 3a. STEADY STATE COMPOSITIONS OF THE CONVENTIONAL COLUMN AFTER GIVING 10% STEP CHANGE (Values in parenthesis are for negative step change).

	x_D	x_B
L	0.9888 (0.8251)	0.1768 (0.0048)
V	0.7650 (0.9897)	0.0035 (0.2368)
f	0.9757 (0.8860)	0.1241 (0.0145)
z	0.9622 (0.8947)	0.1147 (0.0082)

Table 3b. AVERAGE PROCESS GAINS OF THE CONVENTIONAL COLUMN

	x_D	x_B
L	0.008025	0.008431
V	-0.007392	-0.007739
f	0.003375	0.005325
z	0.9320	1.0960

Table 4a. STEADY STATE VALUES OF THE MODIFIED COLUMN AFTER GIVING 10% STEP CHANGE (Values in the parenthesis are for negative step change)

	x_D	x_B	x_c	x_b
L	0.9779 (0.8695)	0.1347 (0.0167)	0.8349 (0.5753)	0.4147 (0.1331)
V	0.8067 (0.9816)	0.0063 (0.2008)	0.4755 (0.8549)	0.0677 (0.4575)
ℓ	0.9661 (0.9110)	0.0949 (0.0275)	0.7924 (0.6337)	0.3605 (0.1847)
ν	0.9136 (0.9628)	0.0246 (0.0978)	0.6402 (0.7785)	0.1700 (0.3661)
f	0.9535 (0.8924)	0.1221 (0.0108)	0.7509 (0.5794)	0.3836 (0.0984)
z	0.9698 (0.8816)	0.1310 (0.0190)	0.8155 (0.5577)	0.4359 (0.1310)

Table 4b. AVERAGE PROCESS GAINS OF THE MODIFIED COLUMN

	x_D	x_B	x_c	x_b
L	0.008377	0.008826	0.01942	0.02106
V	-0.007484	-0.008302	-0.01624	-0.01668
ℓ	0.007838	0.009587	0.02272	0.02501
ν	-0.006999	-0.01041	-0.01967	-0.02790
f	0.003055	0.005565	0.008575	0.01426
z	0.8730	1.1200	2.5780	3.049

are useful in designing an appropriate control scheme for the distillation column. These transfer functions were evaluated by a careful study of the dynamic response of the distillation column.

A 10% positive and negative step change in series as shown in Figure 10 was given for each of the control and disturbance variables, and response of the column is simulated.

The necessary time constants for the dynamic response of the required controlled variables are then identified through a least-square-fit analysis using the subroutines YNORM and ZXSSQ from the IMSL package. First, a 1st order transfer function was tried, and if the fit of the response was not good, then higher order ones were tried. For all the elements of transfer matrix M and some of the transfer matrix P are approximated (for both conventional and modified distillation column) by a 1st order transfer function, as shown in Tables 5 and 6. Sample fits of the dynamic response and approximated transfer functions are given in Figures 11 and 12.

4.3 Feedback Controller Settings

A Proportional-Integral type controller is used for the feedback control of the distillation column. Open-loop transfer functions were used to plot the Bode diagrams to obtain the cross over frequency and amplitude

Table 5. TRANSFER MATRICES FOR THE CONVENTIONAL COLUMN

$$
\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{0.008025}{(5.1986s+1)} & \dfrac{-0.007392}{(6.0143s+1)} \\ \dfrac{0.008431}{(6.4574s+1)} & \dfrac{-0.007734}{(5.5693s+1)} \end{bmatrix} \begin{bmatrix} L \\ V \end{bmatrix}
+ \begin{bmatrix} \dfrac{0.003375}{(28.216s+1)(0.98703s+1)} & \dfrac{0.932}{(6.2765s+1)(0.8811s+1)} \\ \dfrac{0.005325}{(3.4985s+1)(0.2s+1)} & \dfrac{1.096}{(2.6718s+1)\ (2.6779s+1)} \end{bmatrix} \begin{bmatrix} f \\ z \end{bmatrix}
$$

Table 6. TRANSFER MATRICES FOR THE MODIFIED COLUMN

$$
\begin{bmatrix} x_D \\ x_B \\ x_c \\ x_b \end{bmatrix}
=
\begin{bmatrix}
\frac{0.008377}{4.5703s+1} & \frac{-0.007484}{5.8698s+1} & \frac{0.007838}{4.8010s+1} & \frac{-0.006999}{5.6159s+1} \\
\frac{0.008826}{6.6443s+1} & \frac{-0.008322}{5.2739s+1} & \frac{0.009587}{7.2773s+1} & \frac{-0.010413}{6.5944s+1} \\
\frac{0.019417}{3.7583s+1} & \frac{-0.016235}{4.3793s+1} & \frac{0.022717}{3.8825s+1} & \frac{-0.019673}{5.0725s+1} \\
\frac{0.021062}{4.3192s+1} & \frac{-0.016680}{2.6817s+1} & \frac{0.025007}{5.0374s+1} & \frac{-0.027895}{4.0086s+1}
\end{bmatrix}
\begin{bmatrix} L \\ V \\ \ell \\ \nu \end{bmatrix}
+
\begin{bmatrix}
\frac{0.003055}{(19.486s+1)(0.99712s+1)} & \frac{0.8730}{(4.3419s+1)(1.2303s+1)} \\
\frac{0.005565(0.53691s+1)}{(1.8777s+1)(1.8613s+1)} & \frac{1.12(-0.40586s+1)}{(4.1219s+1)(1.3644s+1)} \\
\frac{0.008575}{(12.945s+1)(0.58813s+1)} & \frac{2.578}{(4.8454s+1)} \\
\frac{0.014260}{(3.6452s+1)} & \frac{3.049}{(4.1169s+1)}
\end{bmatrix}
\begin{bmatrix} f \\ z \end{bmatrix}
$$

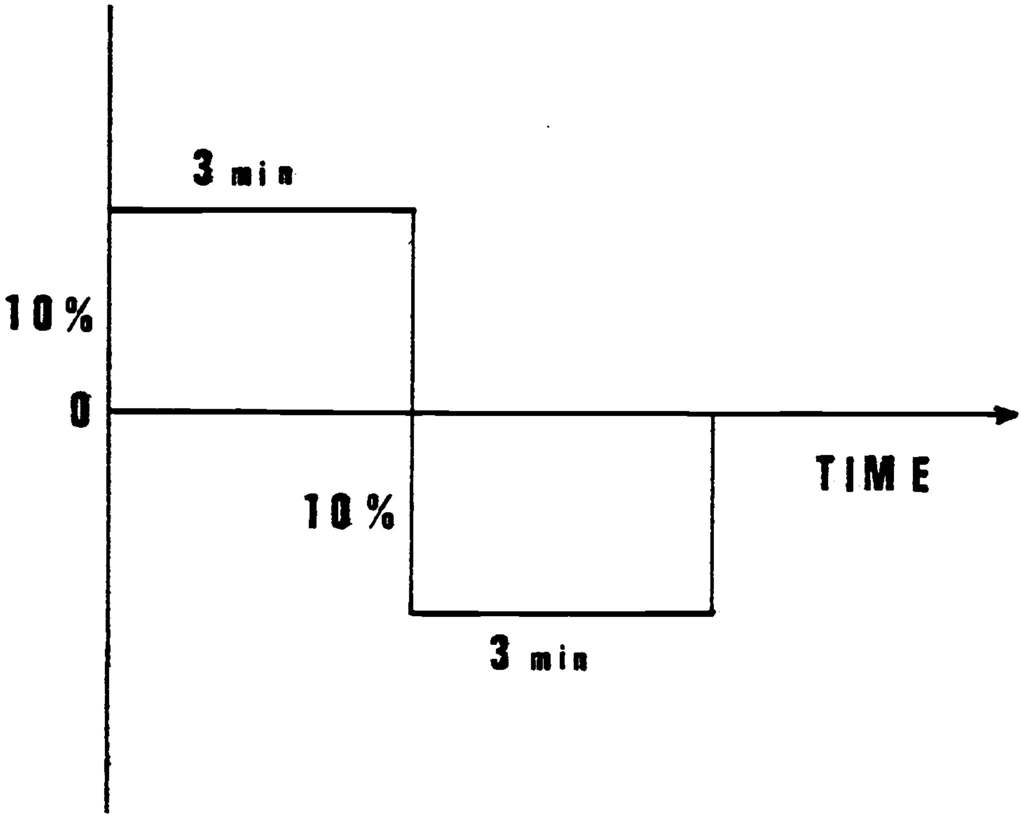

Figure 10. Pulse change used in the feed disturbance.

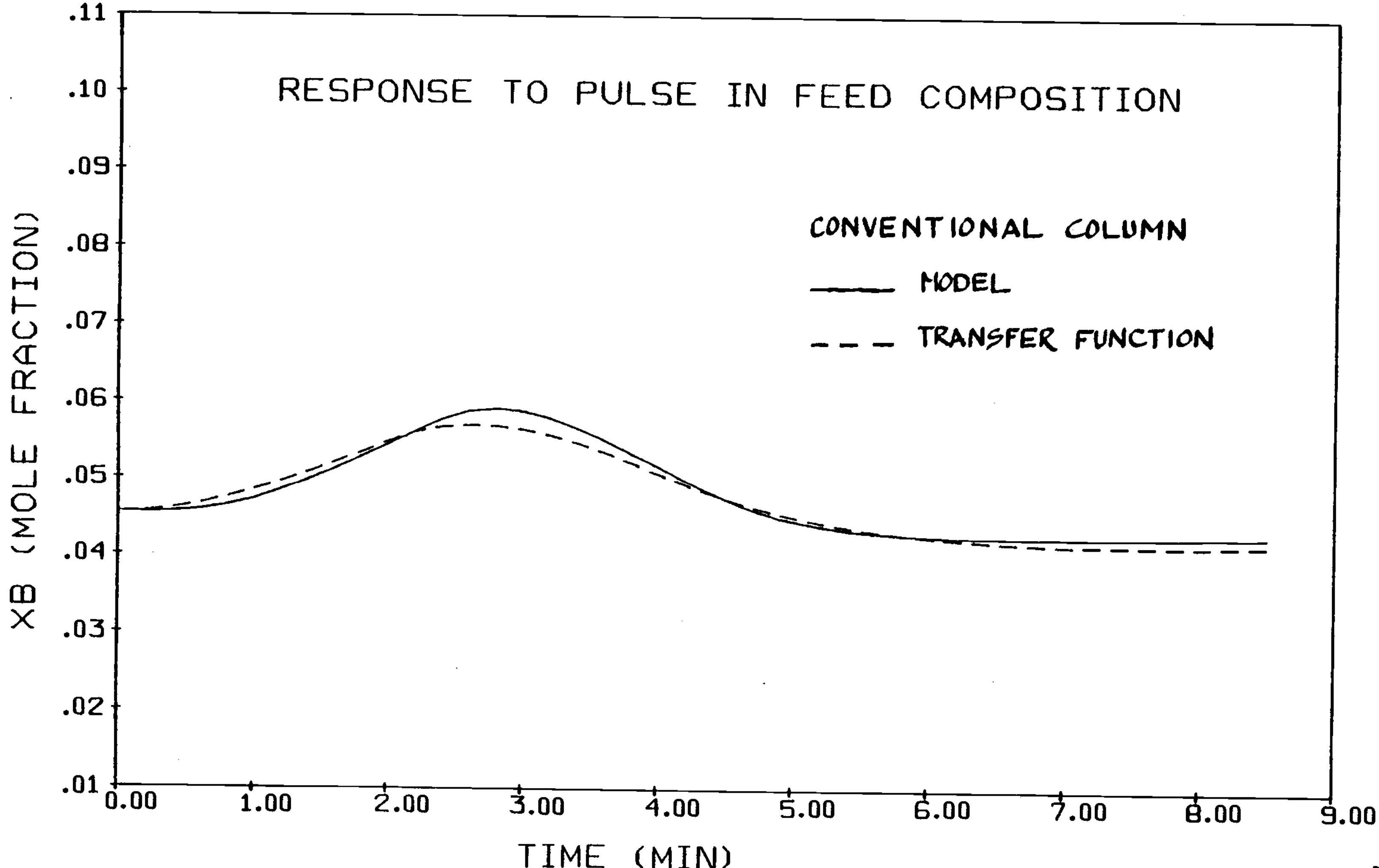

Figure 11. Dynamic response of the conventional column.

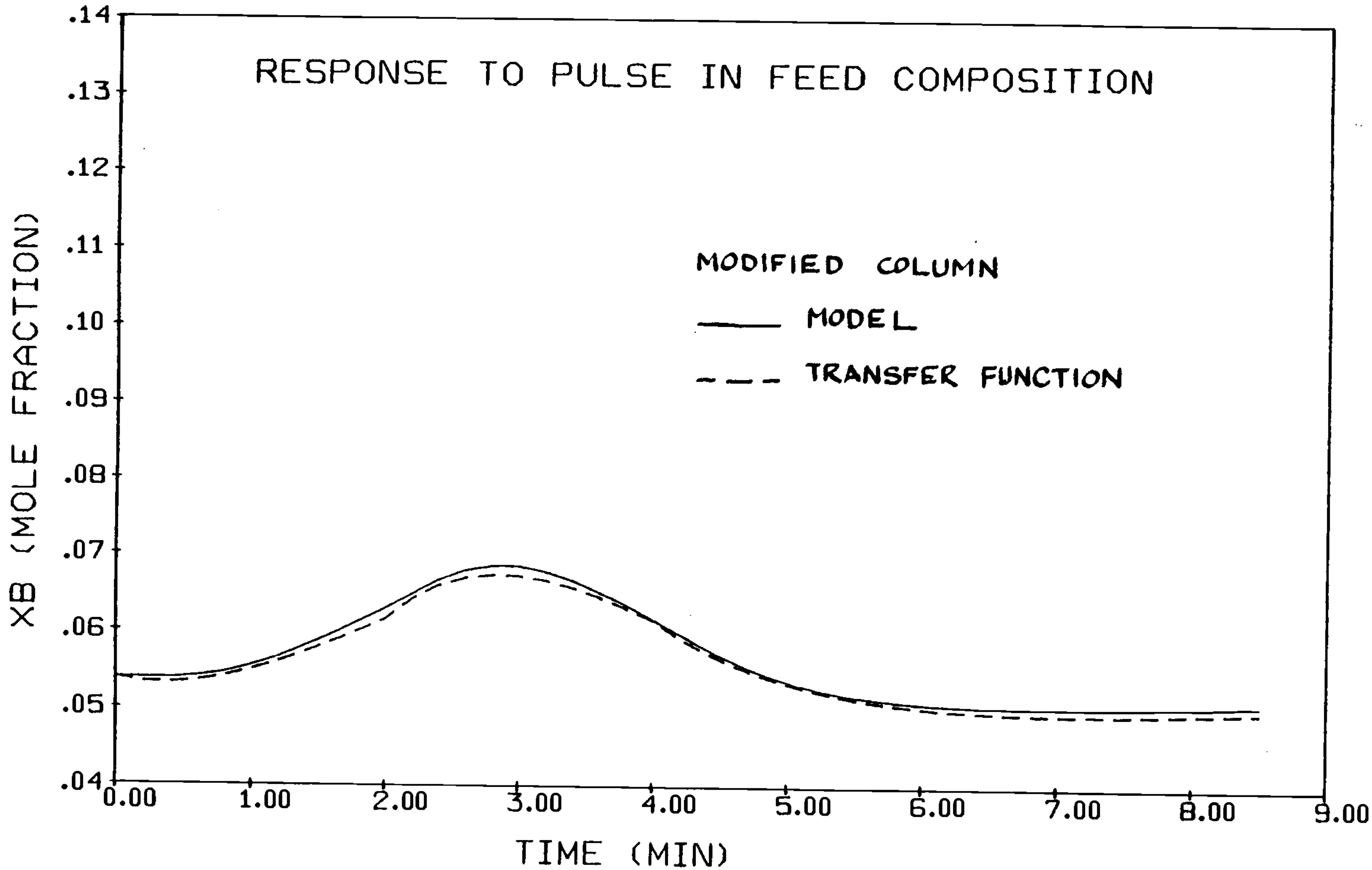

Figure 12. Dynamic response of the modified column.

ratio. Using these values, the feedback controller gain and integral time constant were obtained by Zeigler-Nichols settings (27). These settings were used as a basis for simulation of the control response, and were changed by tuning. The final controller settings chosen after tuning are presented in Table 7. The necessary design calculations and the Bode diagrams are given in Appendix C.

4.4 Feedforward Controller Design

Feedforward loop synthesis consists of developing a steady state model (usually based on material balance), relating controlled variables to disturbance variables, and then applying dynamic compensator to insure the control action is applied at the proper time.

As explained in Chapter 3, two types of feedforward control loops were tried. In one scheme, the intermediate heat exchanger duties were used as the feedforward control variables, and in the second scheme, the main boil-up and reflux rates were used as the feedforward control variables. The necessary transfer functions, which were derived in the previous section, are used to solve the feedforward design Equations 26 and 28 as given in Chapter 3. The algebraic manipulations are given in Appendix D and the final time domain feedforward control elements

Table 7. FEEDBACK CONTROLLER SETTINGS

	x_D	x_B
Conventional Column:		
Gain (K_p)	2300	-2300
Integral Time Constant (τ_I)	0.8	0.8
Modified Column - Case II:		
Gain (K_p)	3000	-3000
Integral Time Constant (τ_I)	0.6	0.6
Modified Column - Case II	x_c	x_b
Gain (K_p)	1200	-1200
Integral Time Constant (τ_I)	0.7	0.7

are as follows.

Case I - feedforward through X_I, U_I:

$$F_{11} = 0.4969 - 1.723\ e^{-0.165t} - 1.1137\ e^{-0.0727t}$$
$$+ 4.3424\ e^{-1.003t} - 447.4\ e^{-0.5574}$$
$$+ 444.0\ e^{-0.533t} + 3.1376\ e^{-0.0513t}$$

$$F_{21} = 0.9875 - 1.096\ e^{-0.165t} - 1.9546\ e^{-0.0727t}$$
$$+ 0.3218\ e^{-1.003t} - 299.9\ e^{-0.557t}$$
$$+ 299.7\ e^{-0.5335t} + 3.4178\ e^{-0.0513t}$$

Case II -feedforward through X_{II}, U_{II}:

$$F_{11} = 4.4038 - 0.019\ e^{-0.179t} - 0.9992\ e^{-0.0182t}$$
$$+ 179.5\ e^{-0.534t} - 180.2\ e^{-0.537t} - 1.9766\ e^{-0.0513t}$$
$$+ 0.1484\ e^{-1.003t}$$

$$F_{21} = 5.4093 - 0.0210\ e^{-0.179t} - 1.1803\ e^{-0.0182t}$$
$$+ 296.8\ e^{-0.534t} - 297.6\ e^{-0.537t} - 2.303\ e^{-0.0513t}$$
$$+ 0.1179\ e^{-1.003t}$$

5.0 SIMULATION

A computer program was developed using the non-linear differential equations model of the distillation column. The column characteristics and feedback controller settings were inputs to the main program. A set of subroutines evaluate the solution of differential equations with necessary feedback, with or without feedforward correction, giving the individual stage compositions and new values of the control and controlled variables as output. All major column disturbances, such as feed rate, heat exchanger duties, and change in feedback controller set points, can be simulated to aid in evaluating not only the control system performance, but also the ability of the distillation system to handle upsets.

The computer program is capable of simulating the dynamic behavior and control response of a distillation column up to 35 actual stages. The limitation being the stiffness of the differential equations to be solved simultaneously, in which case more rigorous and time consuming methods have to be used to overcome this problem.

For a comparative study of the modified and conventional column performances, first a 10% positive step change was given in feed rate and both set points of distillate and bottoms product compositions, so that the columns are brought to new steady states. Then a 10% positive and negative step change in series (Fig. 10) is given in feed rate, so that the columns are brought back to the original steady states. The resulting responses for Case I, where a feedback control through X_I and U_I, and a feedforward control through X_{II} and U_{II} are given in Figures 13 through 28.

Figures 13 and 14 show the variations of distillate and bottoms product compositions respectively, for a step change in distillate composition controller set point. Figures 15 and 16 give the variations in main boil-up and reflux rates respectively, for the same disturbance. Figures 17 through 20 give the variations in the above said variables for step change in bottoms product composition controller set point. It can be clearly seen that the extent of deviation as well as the fluctuations of the compositions and the control variables is much less in the case of the modified column than that of the conventional column.

A step change in feed rate as a disturbance in feed was given and the resulting control responses of the control variables (reflux rate and main boil-up rate) and controlled variables (x_D and x_B) are given in Figures 21 through 24. Whereas Figures 25 through 28 give the control response of the above variables for a positive and negative step change in series. Incorporating the feedforward control for the modified column results in improved response of the control variables (Figures 23 and 24) and very little improvement in the case of controlled variables (Figures 25 and 26), as compared to only feedback control scheme. However, control response of control and controlled variables of the modified column seems to be much better than the conventional column. This is perhaps due to the improved dynamics of the distillation column, where the immediate exchangers help in giving a faster response.

On the other hand, for Case II, where X_{II} and U_{II} are used as feedforward variables, simulation resulted in unstable operation of the column, as shown in Table 8. Here, to control the product compositions, the feedback control variables ℓ and ν, attain negative values. The amount of disturbance was reduced to 5% from 10%, and it was found that (Table 9) the column does exhibit a stable operation.

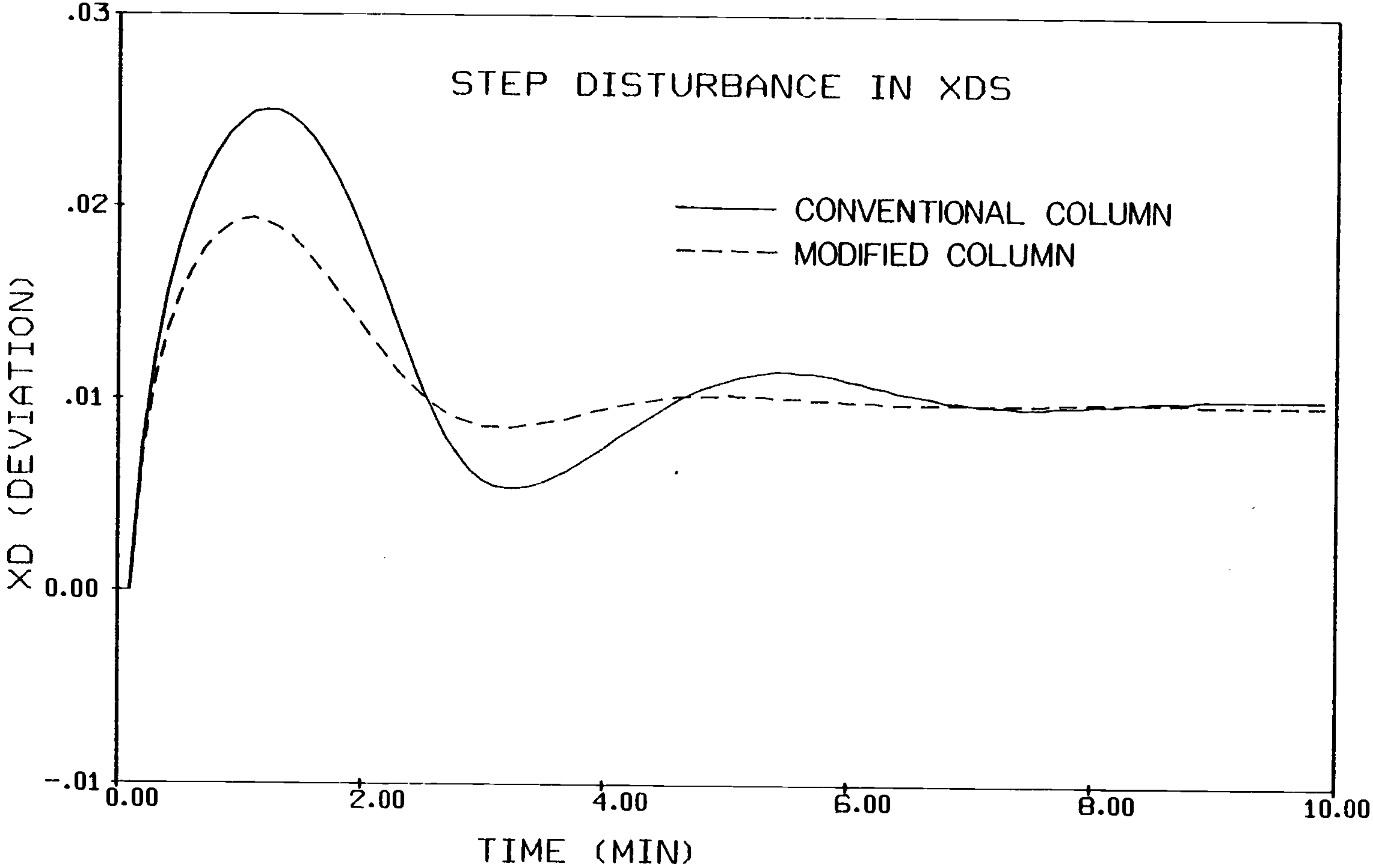

Figure 13. Control response of X_D to a change in X_D^s.

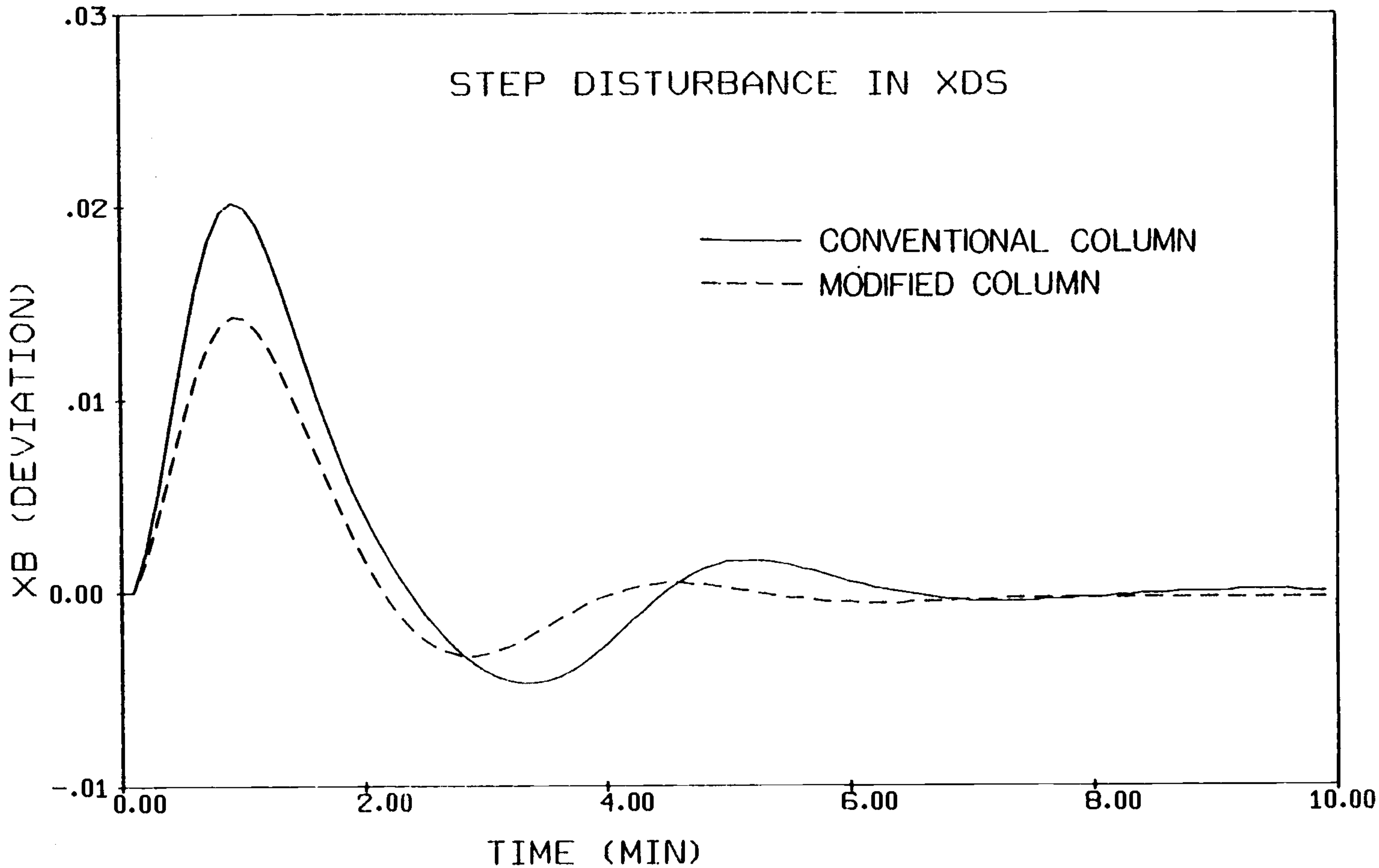

Figure 14. Control response of X_B to a change in X_D^S.

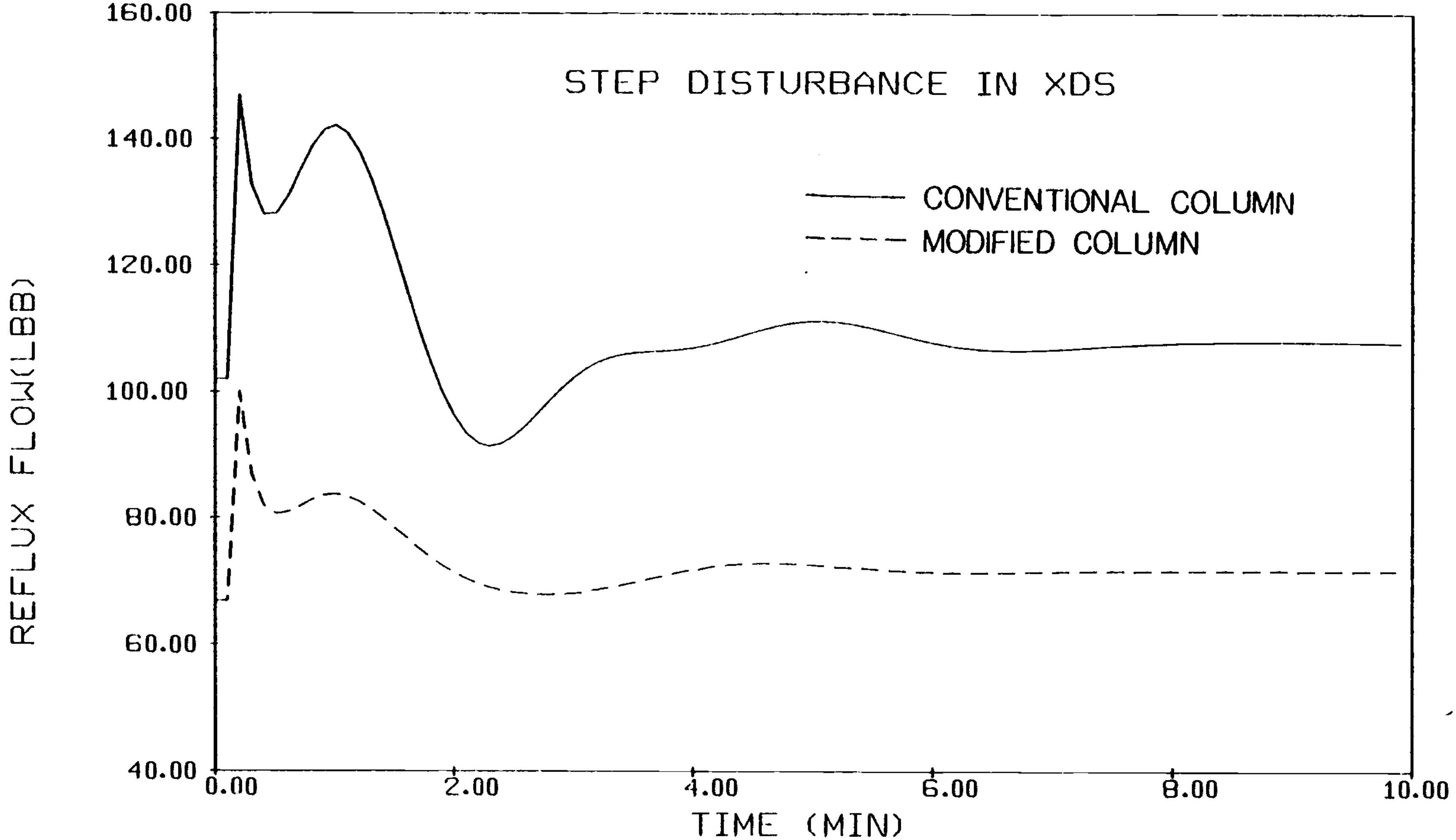

Figure 15. Control response of reflux rate to a change in X_D^S.

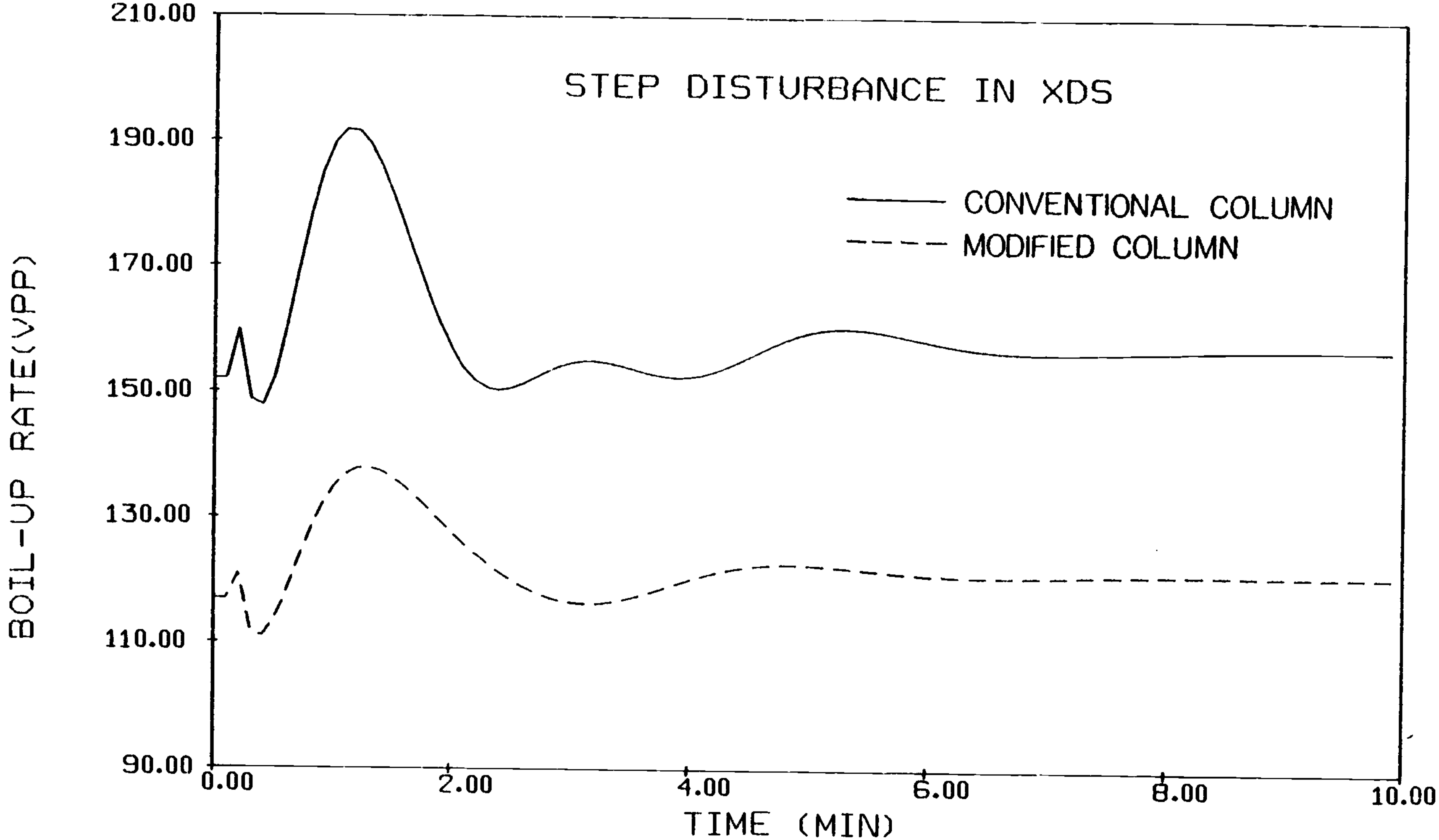

Figure 16. Control response of main boil-up rate to a change in X_D^s.

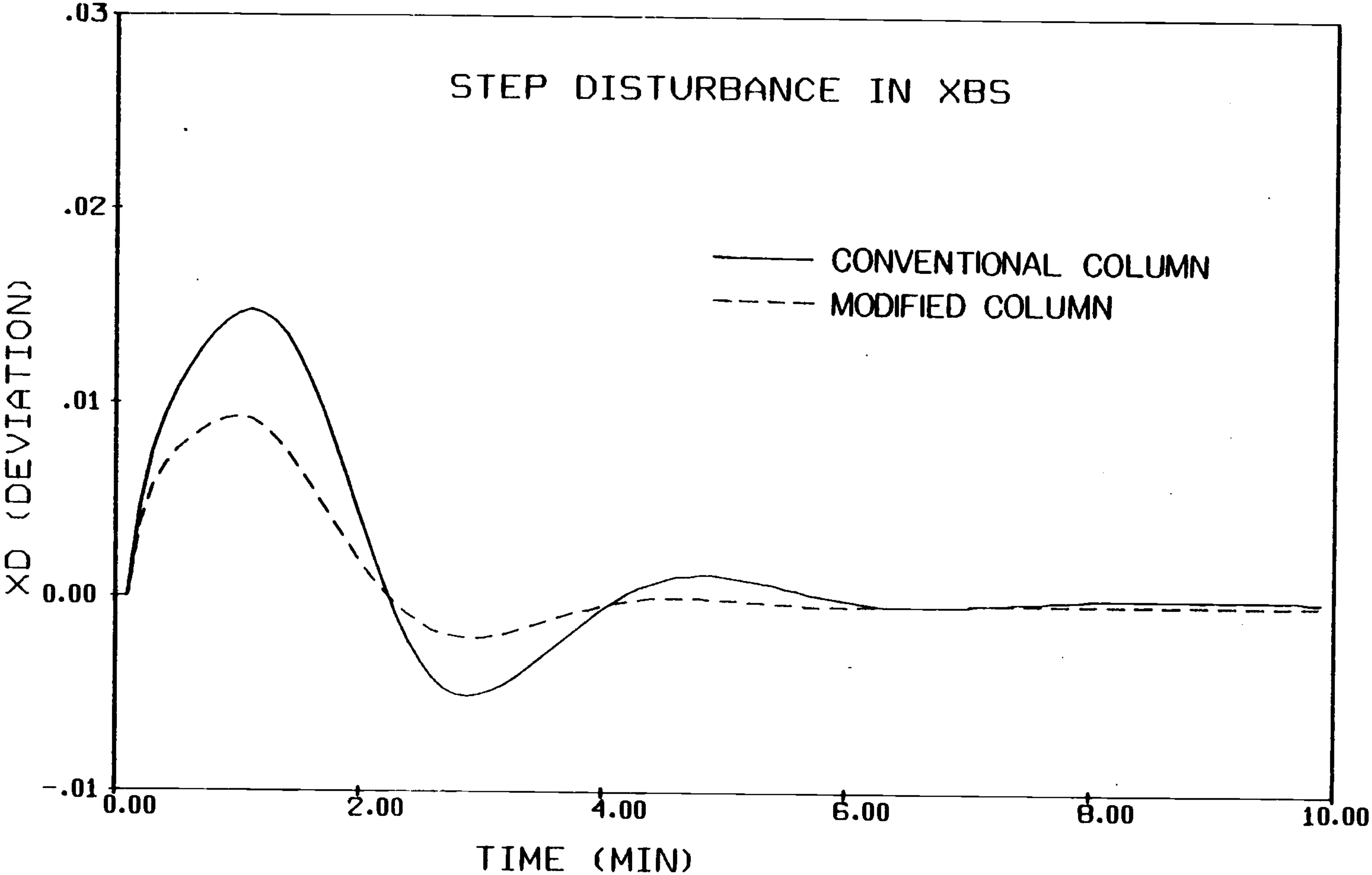

Figure 17. Control response of X_D to a change in X_B^s.

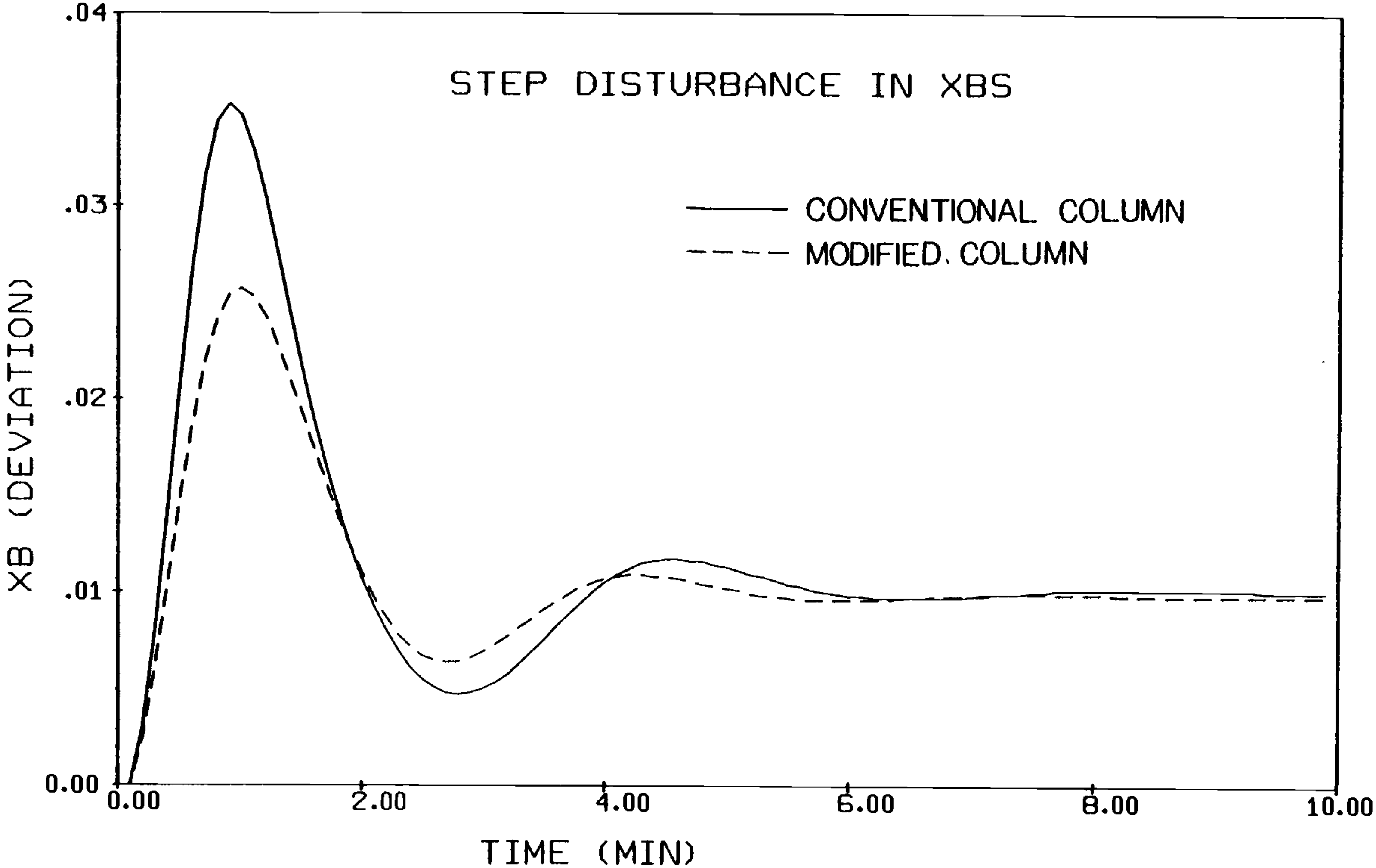

Figure 18. Control response of X_B to a change in X_B^s.

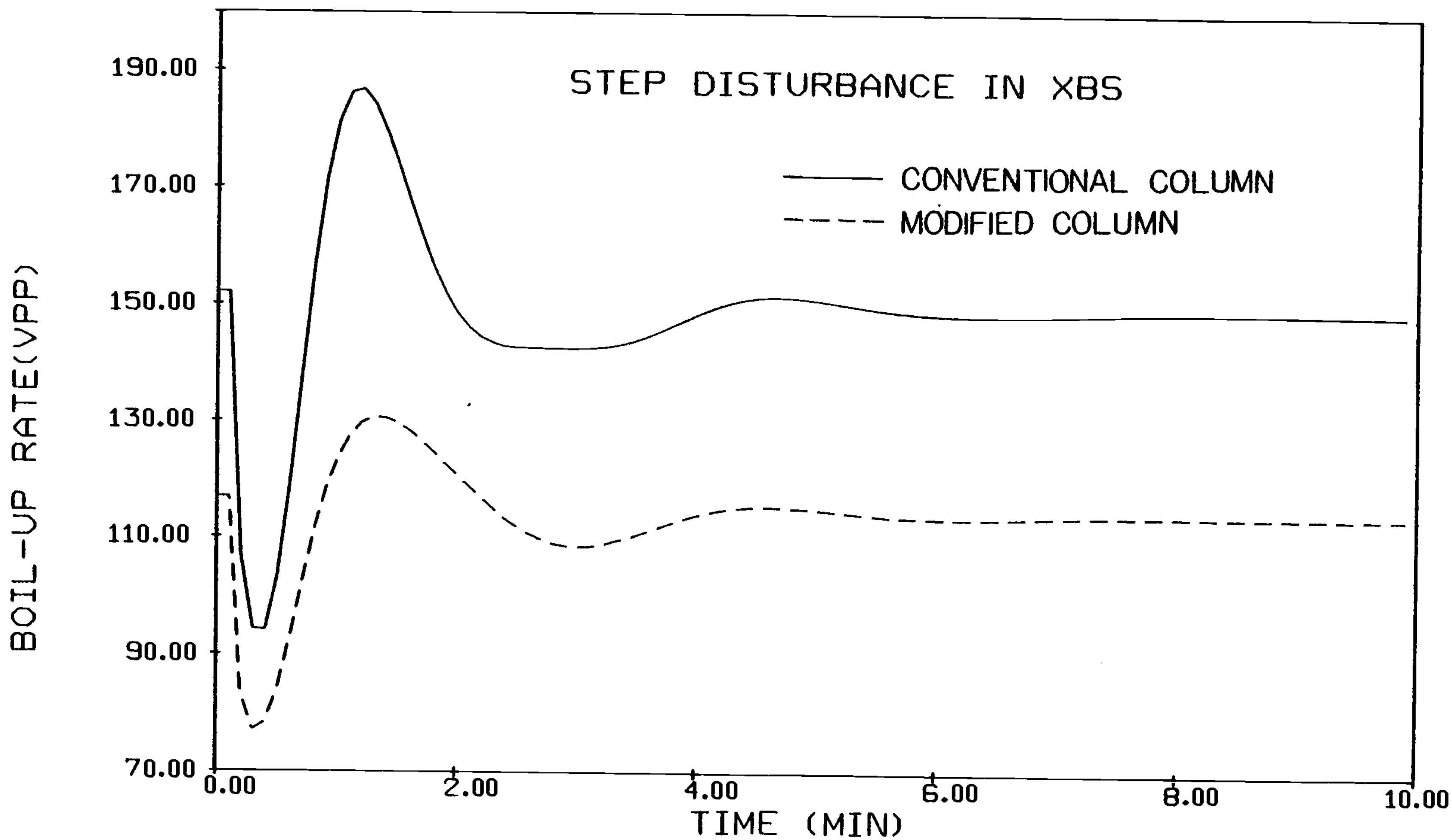

Figure 19. Control response of reflux rate to a change in X_B^s.

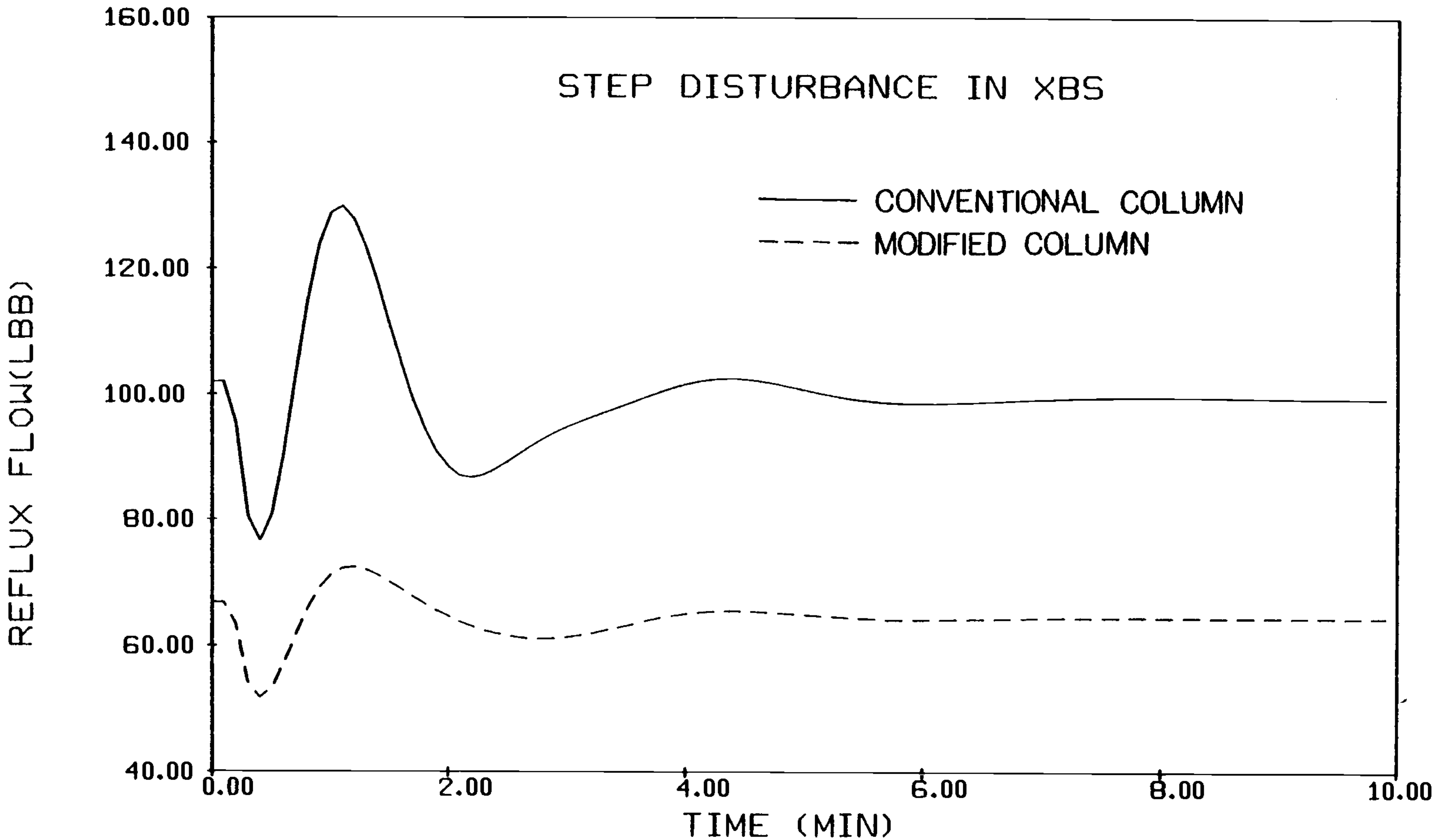

Figure 20. Control response of main boil-up rate to a change in X_B^S.

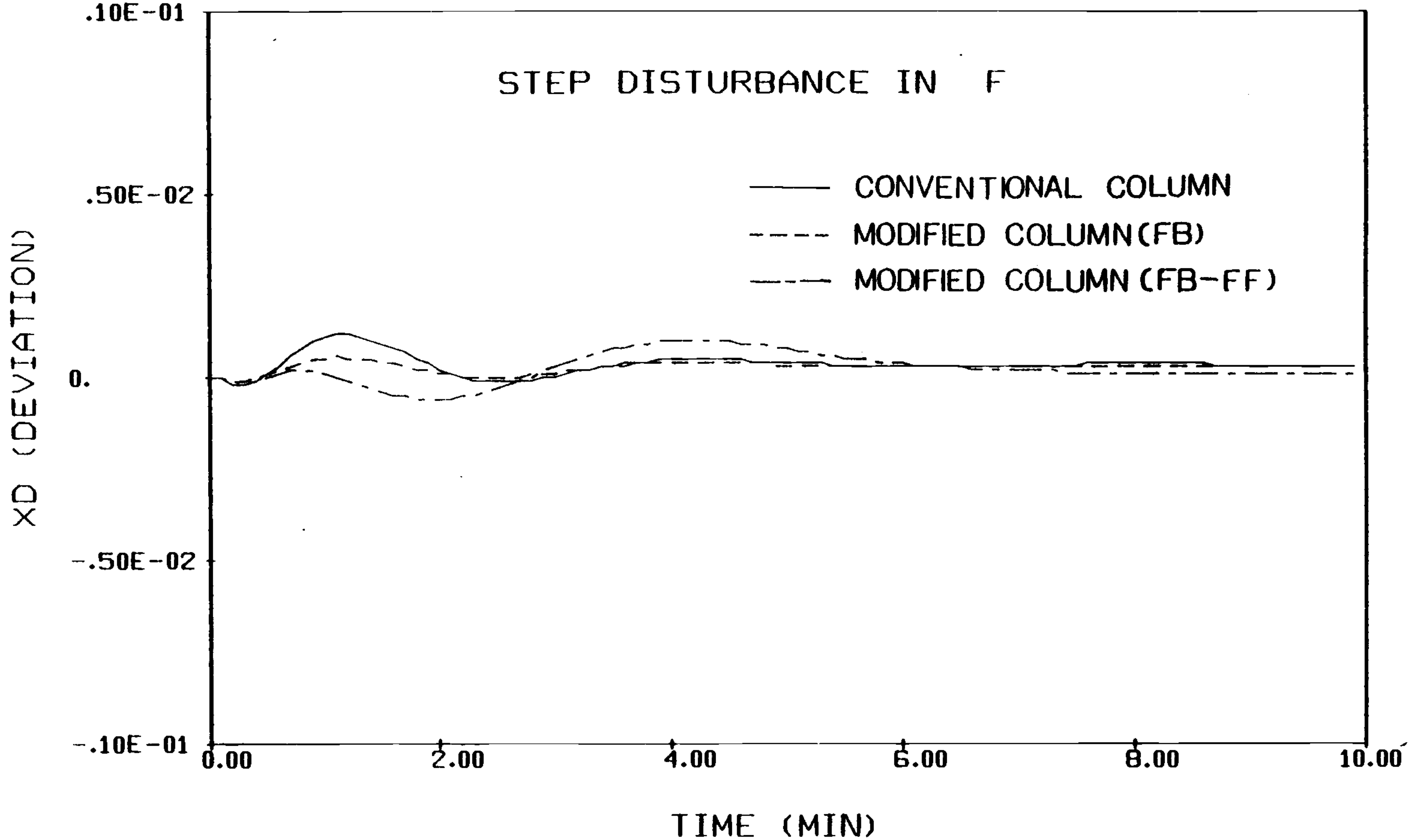

Figure 21. Control response of X_D to a step change in feed rate.

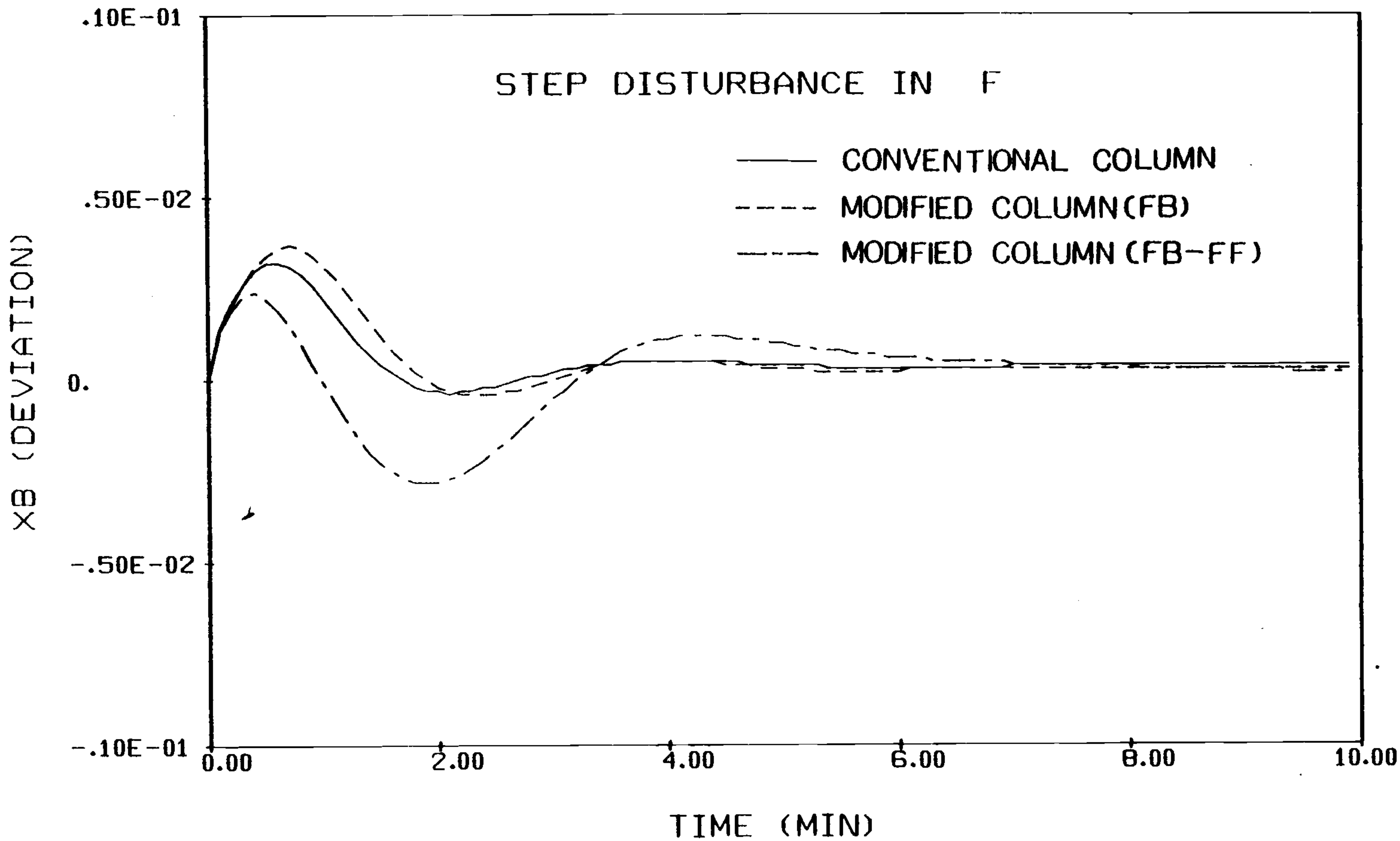

Figure 22. Control response of X_B to a step change in feed rate.

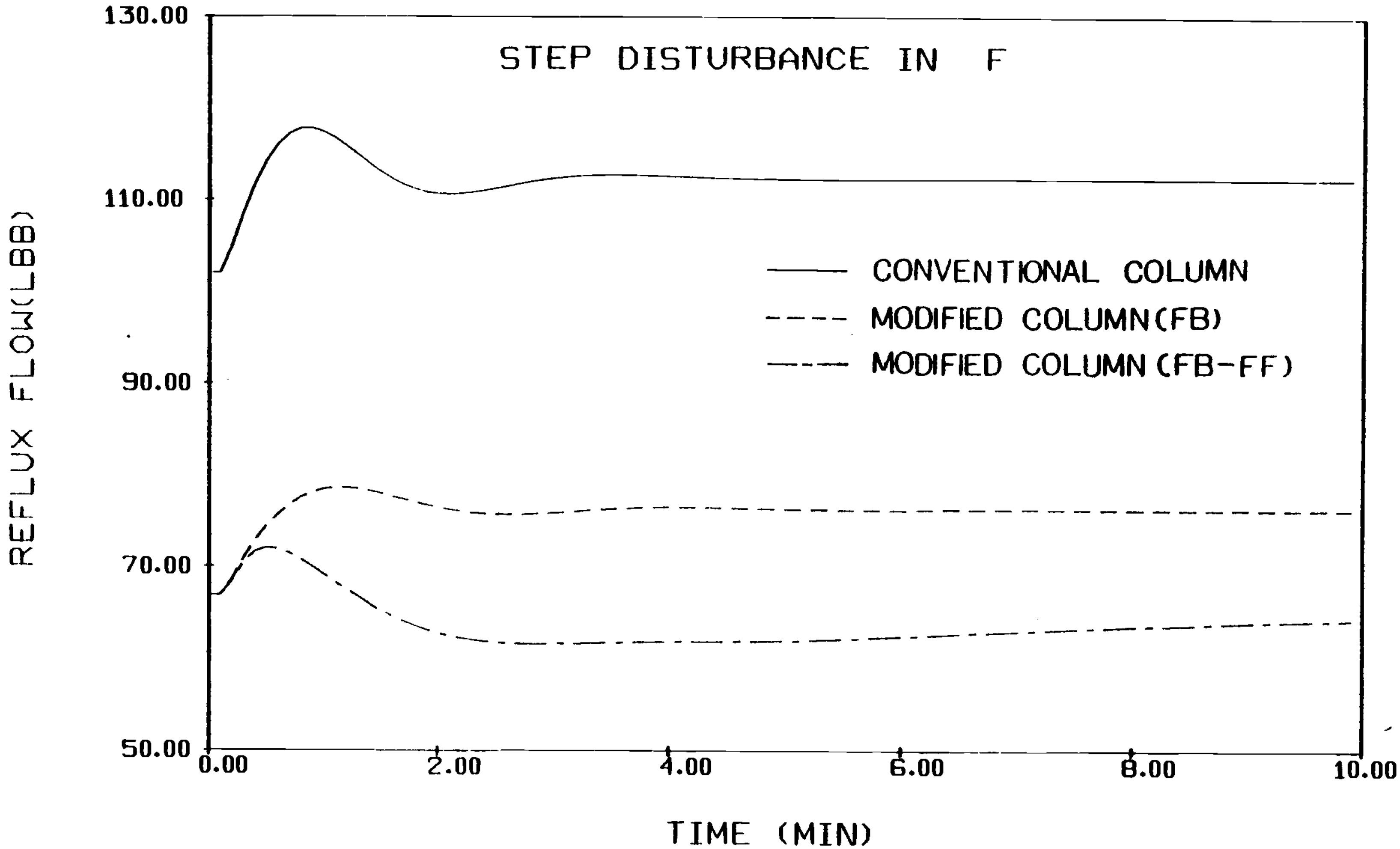

Figure 23. Control response of reflux rate to a step change in feed rate.

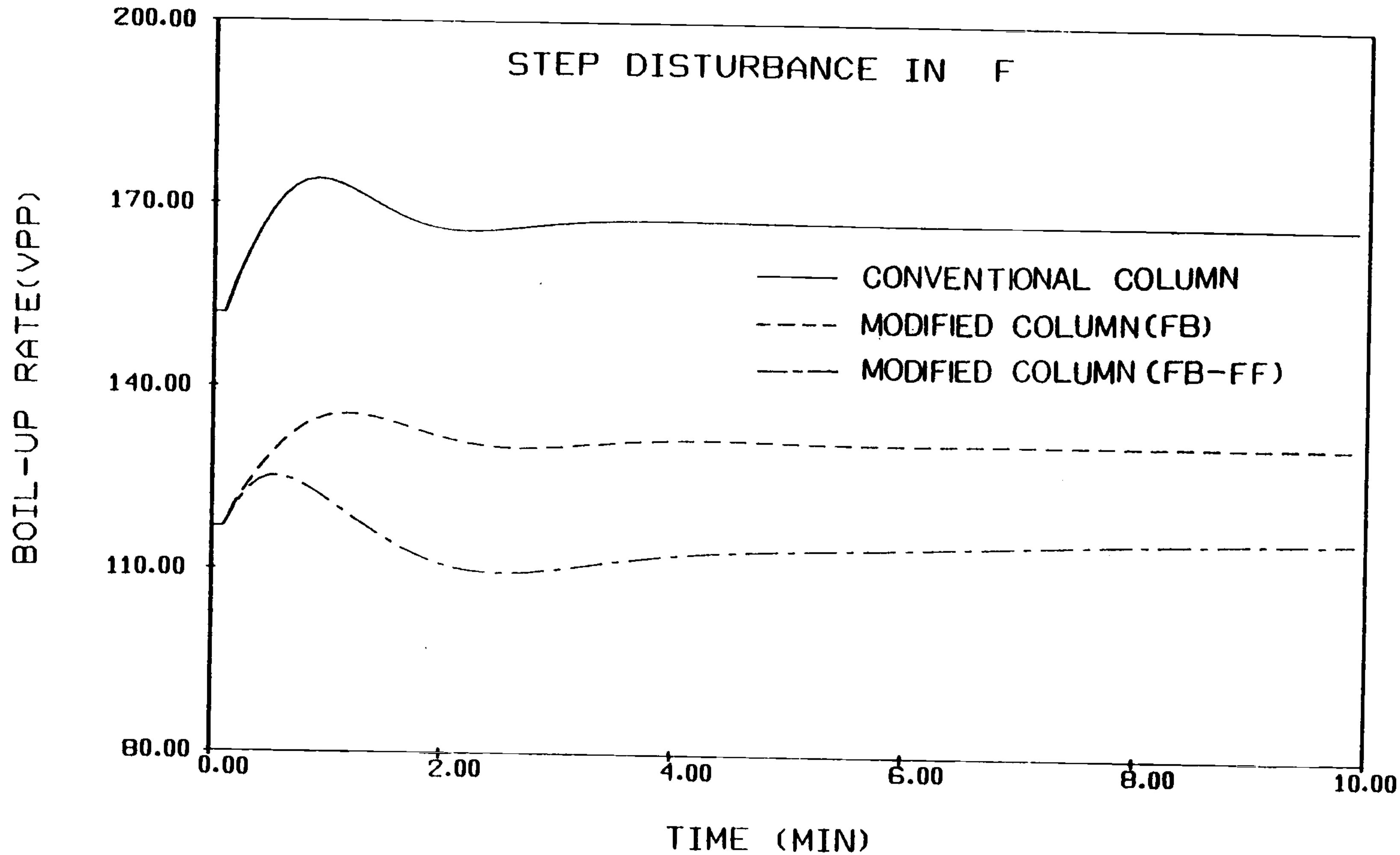

Figure 24. Control response of main boil-up rate to a step change in feed rate.

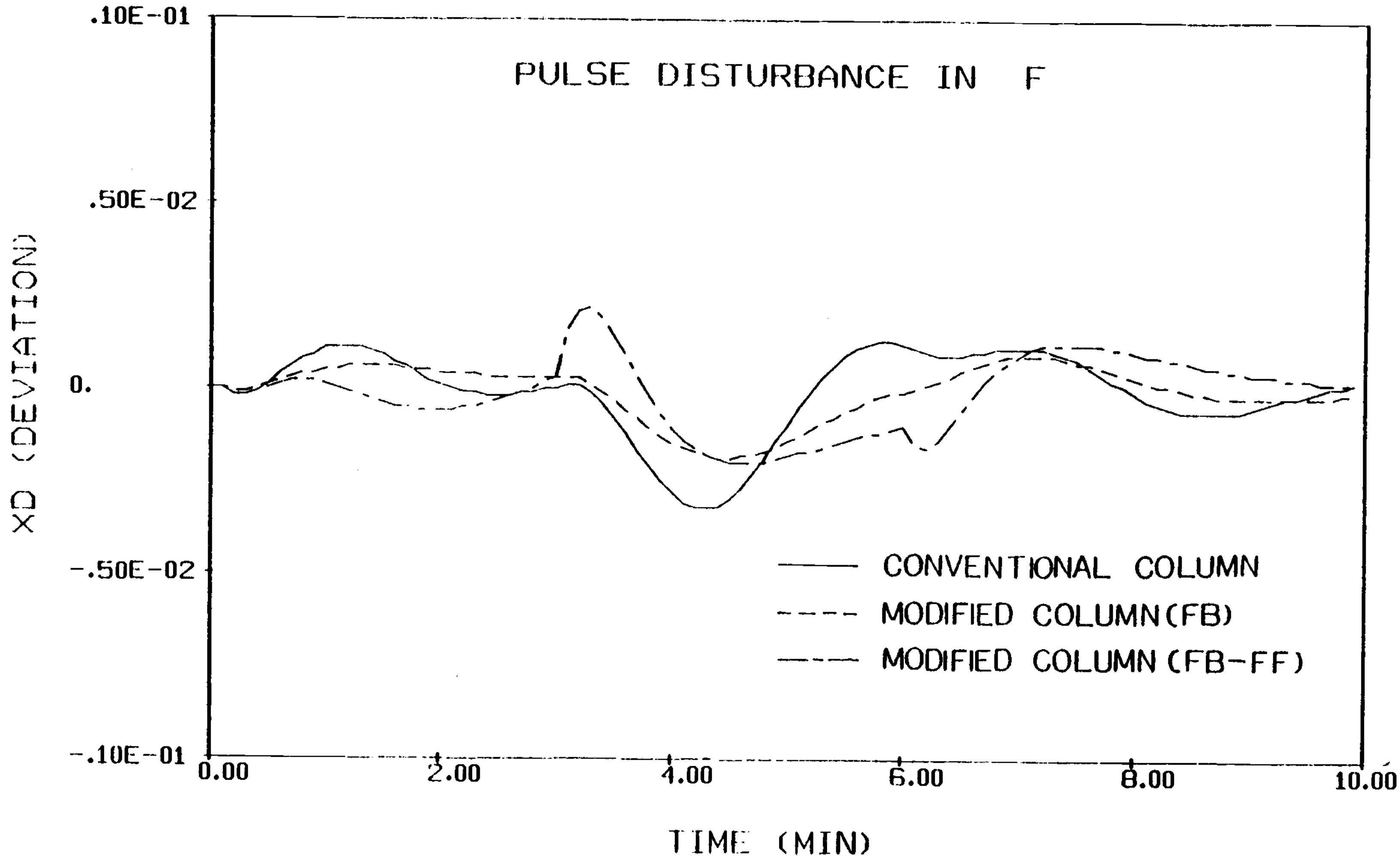

Figure 25. Control response of X_D to a pulse change in feed rate.

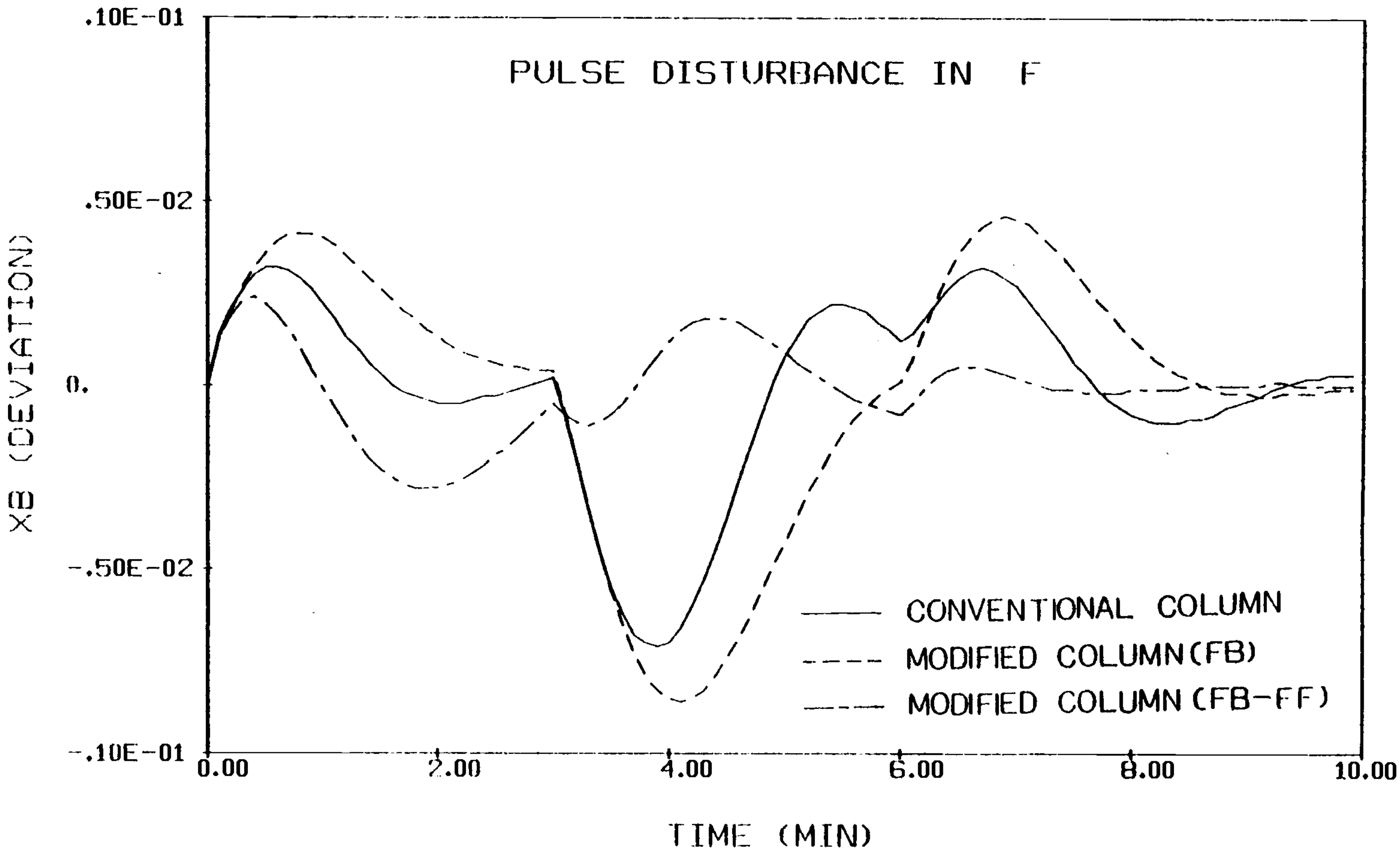

Figure 26. Control response of X_B to a pulse change in feed rate.

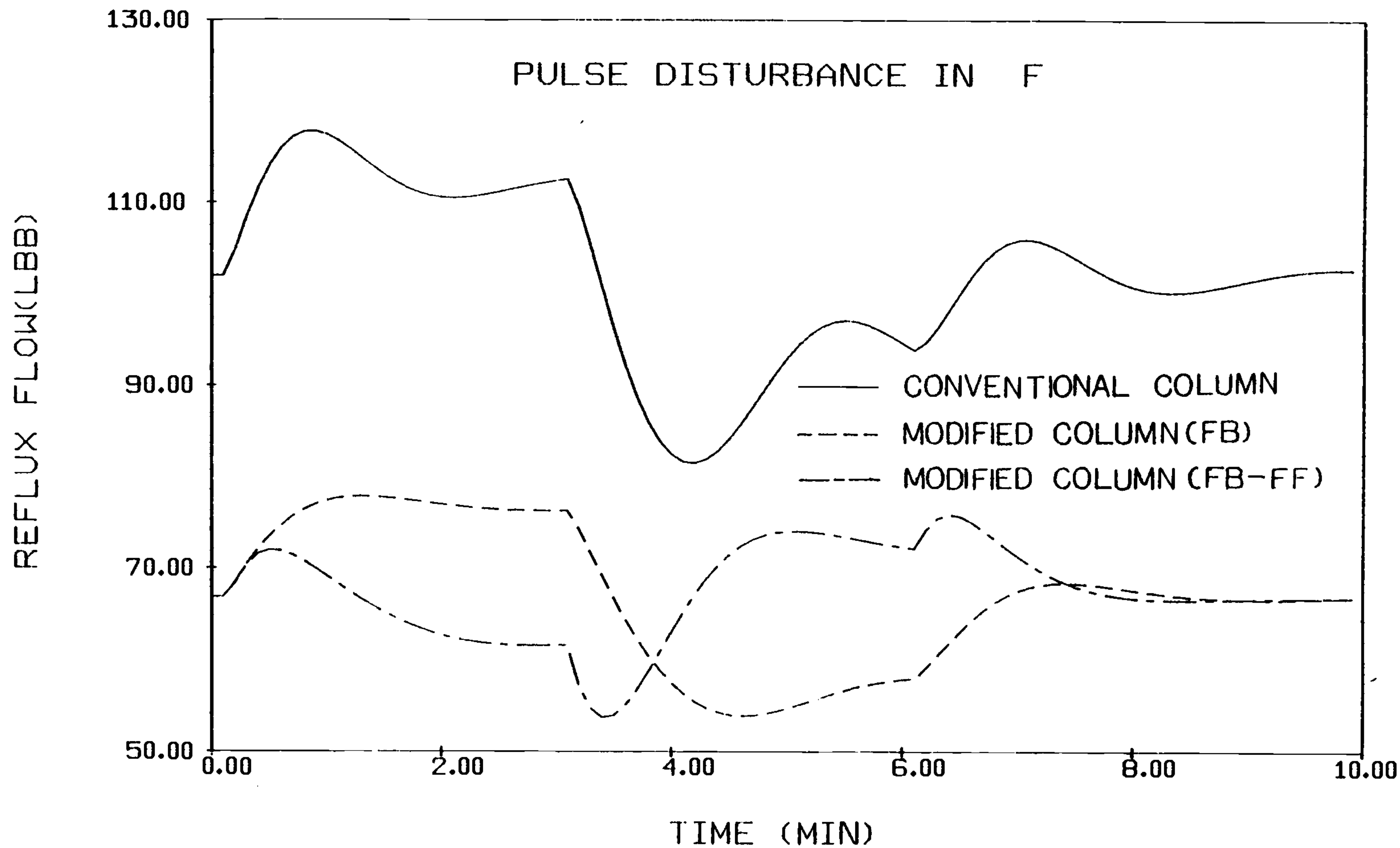

Figure 27. Control response of reflux rate to a pulse change in feed rate.

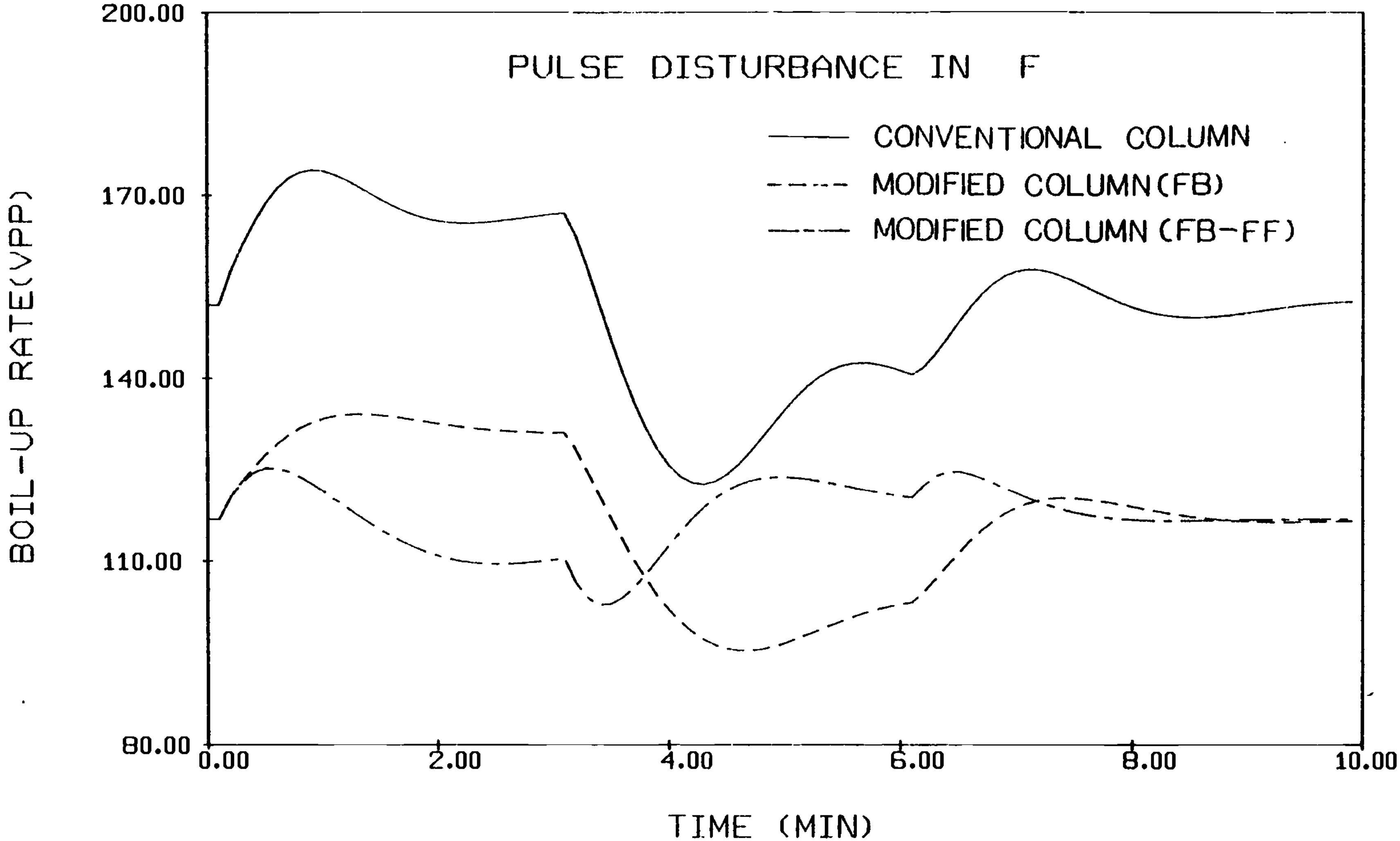

Figure 28. Control response of main boil-up rate to a pulse change in feed rate.

Table 8. SIMULATION RESULTS OF CASE II WITH 10% STEP CHANGE IN FEED RATE

T	L	V	ℓ	ν	ϵ_c	ϵ_b
0.0000	66.8540	116.8540	35.1460	35.1460	0.0000	0.0000
.1000	76.7552	131.1443	35.1460	35.1460	.0002	.0078
.2000	77.5123	132.2704	29.7728	12.1966	.0018	.0143
.3000	78.2168	133.3086	36.4575	26.3344	-.0016	.0021
.4000	78.8722	134.2650	24.6894	14.4326	-.0056	.0061
.5000	79.4816	135.1456	29.5117	20.0847	-.0037	.0031
.6000	80.0483	135.9557	22.0447	11.9144	-.0055	.0063
.7000	80.5751	136.7006	24.8687	14.8631	-.0038	.0048
.8000	81.0647	137.3849	19.8330	9.0812	-.0045	.0070
.9000	81.5197	138.0133	21.5703	10.7741	-.0032	.0060
1.0000	81.9425	138.5898	17.9279	6.4905	-.0035	.0076
1.1000	82.3353	139.1183	19.0527	7.5420	-.0025	.0068
1.2000	82.7004	139.6026	16.2672	4.2317	-.0027	.0079
1.3000	83.0396	140.0461	17.0433	4.9483	-.0018	.0071
1.4000	83.3549	140.4518	14.8217	2.3020	-.0019	.0079
1.5000	83.6480	140.8228	15.3995	2.8460	-.0013	.0072
1.6000	83.9206	141.1618	13.5744	.6788	-.0013	.0077
1.7000	84.1742	141.4715	14.0371	1.1333	-.0008	.0070
1.8000	84.4102	141.7541	12.5071	-.6725	-.0008	.0074
1.9000	84.6299	142.0120	12.9090	-.2528	-.0004	.0067
2.0000	84.8347	142.2471	11.6035	-1.7809	-.0004	.0070
2.1000	85.0257	142.4615	11.9784	-1.3648	-.0000	.0063

Table 9. SIMULATION RESULTS OF CASE II WITH 5% STEP CHANGE IN FEED RATE

T	L	V	ℓ	ν	ε_c	ε_b
0.0000	66.8540	116.8540	35.1460	35.1460	0.0000	0.0000
.1000	71.8046	123.9991	35.1460	35.1460	.0001	.0039
.2000	72.1832	124.5622	32.5931	24.7915	.0009	.0071
.3000	72.5354	125.0813	34.5286	29.1133	-.0005	.0021
.4000	72.8631	125.5595	30.9745	25.8071	-.0021	.0028
.5000	73.1678	125.9998	31.1048	26.1722	-.0018	.0020
.6000	73.4512	126.4049	29.3892	24.3577	-.0020	.0026
.7000	73.7146	126.7773	28.9763	23.8526	-.0016	.0025
.8000	73.9594	127.1195	28.0134	22.7025	-.0015	.0028
.9000	74.1868	127.4336	27.5509	22.0799	-.0012	.0028
1.0000	74.3982	127.7219	26.9272	21.2802	-.0010	.0029
1.1000	74.5947	127.9862	26.5227	20.7327	-.0007	.0028
1.2000	74.7772	128.2283	26.0766	20.1543	-.0005	.0028
1.3000	74.9468	128.4500	25.7403	19.7158	-.0004	.0027
1.4000	75.1045	128.6529	25.4054	19.2978	-.0003	.0026
1.5000	75.2510	128.8384	25.1296	18.9629	-.0001	.0024
1.6000	75.3873	129.0079	24.8704	18.6628	-.0001	.0023
1.7000	75.5141	129.1627	24.6487	18.4190	-.0000	.0021
1.8000	75.6321	129.3041	24.4470	18.2101	.0000	.0019
1.9000	75.7420	129.4330	24.2728	18.0426	.0001	.0017
2.0000	75.8443	129.5506	24.1183	17.9060	.0001	.0016
2.1000	75.9398	129.6578	23.9858	17.8014	.0001	.0014
2.2000	76.0290	129.7555	23.8713	17.7229	.0001	.0013
2.3000	76.1123	129.8445	23.7751	17.6697	.0002	.0011
2.4000	76.1902	129.9256	23.6950	17.6379	.0002	.0010

2.068 CP SECONDS EXECUTION TIME.

6. CONCLUSIONS

Based on the computer simulation study on a binary conventional and a modified distillation column, it was observed that the control response is better in the latter case. When the set points of the feedback controllers (both x_D and x_B) were altered, the products compositions (x_D and x_B) attain the new steady states quicker (about 30%) and with smaller fluctuations (about 40%) in the modified column than in the conventional column. Similar behavior was also observed with the reflux and the main boil-up rates. When a 10% step disturbance, as well as pulse disturbance was given in the feed rate, the maximum deviation from the steady state values of the control variables (reflux and main boil-up rates) were smaller by about 40% and attained their new steady states at a relatively faster rate in the modified column than in the conventional column. Little improvement in the control response of the products' compositions of the modified column was seen when a 10% step change was given in the feed rate. When the system was brought back to the original steady state after giving a pulse disturbance in feed rate, there was considerable improvement in the response of the controlled variables.

It is interesting to note that the feedback/feedforward control scheme for the modified column exhibited a better control response for x_B than the feedback control policy alone, whereas only feedback control was better for x_D. The use of saturated liquid feed, which affects the bottom portion of the column more than the top portion, may have caused this kind of behavior. Also, the responses of the control variables were closer to the steady states (but showed more fluctuation) when feedback/feedforward control was used, as compared to the feedback control alone.

On the other hand, for Case II, where side heat exchangers were used as the feedforward control variables, the simulation resulted in unstable operation of the column. When the disturbance was reduced to 5% from 10%, the column performance resulted in a stable operation; this indicates that these feed forward control variables are more sensitive to disturbance in feed.

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APPENDICES

APPENDIX A

To avoid the rigorous solution of the non-linear differential equation model of a binary distillation column, often a linearized model is used to control law computations. Such a linear model is obtained by linearizing the non-linear model about the desired steady state. Thus, a linear model of a typical binary distillation column can be represented by

$$x = Ax + Bu + Wd \tag{1}$$

where u and d are control and disturbance variables, respectively. A, B and W matrices are independent of changes in disturbance and control variables and entirely dependent upon the steady state conditions around which the model is linearized. Thus, these matrices remain constant throughout the process, as long as the initial steady state is not changed during the simulation study. Note that matrix A is a tri-diagonal matrix. Taking Lapace transformation of Equation 1, we get

$$x = [sI-A]^{-1} Bu + [sI-A]^{-1} Wd \tag{2}$$

The necessary time constants representing the dynamic behavior of the distillation column are easily obtained, once the roots of the determinant (sI-A) are determined.

These time constants are nothing but the reciprocals of the poles which are the roots of the above determinant. These poles are the eigen values of A(23). So, once the eigen values of A are determined, appropriate transfer functions and control policy could be designed.

A typical binary distillation process with 15 ideal stages was used to test the above linearized model. The subroutine EQRT2S from the IMSL package was used to find the eigen values of matrix A.

The eigen values of A could not be determined due to the difficulty encountered in finding the inverse of A. So, without the eigen values of A, the alternative way of finding the inverse functions is to go through rigorous non-linear differential equations treatment. A computer output giving the individual elements of matrices A, B and D are given in Table 1.

Table 1. CO-EFFICIENT MATRICES OF LINEAR MODEL

MATRIX A

-.69425	.60000	0	0	0	0	0	0	0	0	0	0	0	0	0
.39425	-.94494	.60000	0	0	0	0	0	0	0	0	0	0	0	0
0	.34494	-.91909	.60000	0	0	0	0	0	0	0	0	0	0	0
0	0	.31909	-.95707	.65000	0	0	0	0	0	0	0	0	0	0
0	0	0	.35707	-.99268	.65000	0	0	0	0	0	0	0	0	0
0	0	0	0	.34268	-.98529	.65000	0	0	0	0	0	0	0	0
0	0	0	0	0	.33529	-.98153	.65000	0	0	0	0	0	0	0
0	0	0	0	0	0	.33153	-.97963	.15000	0	0	0	0	0	0
0	0	0	0	0	0	0	.32963	-.47813	.15000	0	0	0	0	0
0	0	0	0	0	0	0	0	.32813	-.47488	.15000	0	0	0	0
0	0	0	0	0	0	0	0	0	.32488	-.46791	.15000	0	0	0
0	0	0	0	0	0	0	0	0	0	.31791	-.41041	.10000	0	0
0	0	0	0	0	0	0	0	0	0	0	.26041	-.35666	.10000	0
0	0	0	0	0	0	0	0	0	0	0	0	.25666	-.34737	.10000
0	0	0	0	0	0	0	0	0	0	0	0	0	.24737	-.25077

MATRIX B

.07940	-.15877	.07940	-.07940
.04880	-.09760	.04880	-.04880
.02690	-.05397	.02690	-.02690
.02710	-.02802	.02710	-.18325
.01460	-.02708	.01460	-.02708
.00760	-.01414	.00760	-.01414
.00390	-.00724	.00390	-.00724
.00310	-.00368	.00310	-.00368
.00680	-.00291	.00680	-.00291
.01490	-.00634	.01490	-.00634
.03170	-.01368	.03170	-.01368
.01030	-.02815	.17679	-.02815
.02650	-.00888	.00888	-.00888
.06650	-.02226	.02226	-.02226
.15705	-.05243	.05243	-.05243

MATRIX D

.07940	0
.04880	0
.02690	0
.02710	0
.01460	0
.00760	0
.00390	0
-.55000	.50000
0	0
0	0
0	0
0	0
0	0
0	0
0	0

APPENDIX B

A computer output, to evaluate the steady state gain of the controlled variables with respect to change in reflux rate, is given here for the distillation column with side heat exchangers. The output contains the new steady state values of the controlled variables, with a positive as well as a negative 10% step change in reflux rate. Note that, the stage and reboiler hold-ups are fixed at 1.0 mole each rather than 10.0 moles. This is done to reduce the computation time.

```
RELATIVE VOLATILITY                      2.000
NUMBER OF PLATES                        20
FEED PLATE(FROM BOTTOM)                 11
INTERMEDIATE REBOILER PLATE              6
INTERMEDIATE CONDENSOR PLATE            16

FEED COMPOSITION                          .500
TOP PRODUCT COMPOSITION                   .946
BOTTOMS PRODUCT COMPOSITION               .054

FEED RATE, MOLES/MIN                   100.000
DISTILLATE RATE, MOLES/MIN              50.000
BOTTOMS PRODUCT RATE, MOLES/MIN         50.000
REFLUX RATE, MOLES/MIN                  66.854
MAIN BOIL-UP RATE, MOLES/MIN           116.854
INTERM. BOIL-UP RATE, MOLES/MIN         35.146
INTERM. COND. LOAD. MOLES/MIN           35.146

REFLUX RATIO                             2.040 * ?
REFLUX/MINIMUM REFLUX                    1.200
PLATE HOLD UP. MOLES/PLATE               1.000
REBOILER HOLD UP, MOLES                  1.000


THE CHANGES IN LOAD ARE
DF    =      0
DZ    =      0
DLBB  = -6.685
DVPP  =      0
DSL   =      0
DSV   =      0
```

TIME(MIN)	XB	XIB	XF	XIC	XD
0	.0538	.2741	.4956	.7237	.9459
.200	.0336	.2109	.4708	.6687	.9221
.400	.0248	.1736	.4532	.6322	.9042
.600	.0206	.1537	.4420	.6079	.8908
.800	.0187	.1435	.4354	.5930	.8816
1.000	.0177	.1382	.4319	.5845	.8760
1.200	.0172	.1356	.4300	.5799	.8728
1.400	.0170	.1343	.4291	.5775	.8711
1.600	.0168	.1336	.4286	.5763	.8702
1.800	.0168	.1333	.4284	.5757	.8698
2.000	.0167	.1331	.4282	.5753	.8695

THE NEW STEADY STATE CONDITIONS ARE

RELATIVE VOLATILITY	2.000
NUMBER OF PLATES	20
FEED PLATE(FROM BOTTOM)	11
INTERMEDIATE REBOILER PLATE	6
INTERMEDIATE CONDENSOR PLATE	16
FEED COMPOSITION	.500
TOP PRODUCT COMPOSITION	.870
BOTTOMS PRODUCT COMPOSITION	.017
FEED RATE, MOLES/MIN	100.000
DISTILLATE RATE, MOLES/MIN	56.685
BOTTOMS PRODUCT RATE, MOLES/MIN	43.315
REFLUX RATE, MOLES/MIN	60.169
MAIN BOIL-UP RATE, MOLES/MIN	116.854
INTERM. BOIL-UP RATE, MOLES/MIN	35.146
INTERM. COND. LOAD, MOLES/MIN	35.146
REFLUX RATIO	1.061
REFLUX/MINIMUM REFLUX	1.200
PLATE HOLD UP, MOLES/PLATE	1.000
REBOILER HOLD UP, MOLES	1.000

14.013 CP SECONDS EXECUTION TIME

RELATIVE VOLATILITY	2.000
NUMBER OF PLATES	20
FEED PLATE(FROM BOTTOM)	11
INTERMEDIATE REBOILER PLATE	6
INTERMEDIATE CONDENSOR PLATE	16
FEED COMPOSITION	.500
TOP PRODUCT COMPOSITION	.946
BOTTOMS PRODUCT COMPOSITION	.054
FEED RATE, MOLES/MIN	100.000
DISTILLATE RATE, MOLES/MIN	50.000
BOTTOMS PRODUCT RATE, MOLES/MIN	50.000
REFLUX RATE, MOLES/MIN	66.854
MAIN BOIL-UP RATE. MOLES/MIN	116.854
INTERM. BOIL-UP RATE, MOLES/MIN	35.146
INTERM. COND. LOAD. MOLES/MIN	35.146
REFLUX RATIO	2.040
REFLUX/MINIMUM REFLUX	1.200
PLATE HOLD UP, MOLES/PLATE	1.000
REBOILER HOLD UP, MOLES	1.000

THE CHANGES IN LOAD ARE

DF	=	0
DZ	=	0
DLBB	=	6.685
DVPP	=	0
DSL	=	0
DSV	=	0

TIME(MIN)	XB	XIB	XF	XIC	XD
0	.0538	.2741	.4956	.7237	.9459
.200	.0823	.3370	.5191	.7772	.9634
.400	.1044	.3749	.5319	.8065	.9711
.600	.1188	.3952	.5385	.8213	.9747
.800	.1269	.4054	.5417	.8284	.9764
1.000	.1310	.4103	.5433	.8319	.9772
1.200	.1330	.4127	.5440	.8335	.9776
1.400	.1339	.4138	.5444	.8343	.9778
1.600	.1344	.4143	.5446	.8347	.9779
1.800	.1346	.4145	.5446	.8348	.9779
2.000	.1347	.4147	.5447	.8349	.9779

THE NEW STEADY STATE CONDITIONS ARE

RELATIVE VOLATILITY	2.000
NUMBER OF PLATES	20
FEED PLATE(FROM BOTTOM)	11
INTERMEDIATE REBOILER PLATE	6
INTERMEDIATE CONDENSOR PLATE	16
FEED COMPOSITION	.500
TOP PRODUCT COMPOSITION	.978
BOTTOMS PRODUCT COMPOSITION	.135
FEED RATE, MOLES/MIN	100.000
DISTILLATE RATE, MOLES/MIN	43.315
BOTTOMS PRODUCT RATE, MOLES/MIN	56.685
REFLUX RATE, MOLES/MIN	73.539
MAIN BOIL-UP RATE, MOLES/MIN	116.854
INTERM. BOIL-UP RATE, MOLES/MIN	35.146
INTERM. COND. LOAD, MOLES/MIN	35.146
REFLUX RATIO	1.698
REFLUX/MINIMUM REFLUX	1.200
PLATE HOLD UP, MOLES/PLATE	1.000
REBOILER HOLD UP, MOLES	1.000

12.089 CP SECONDS EXECUTION TIME

APPENDIX C

Conventional Column - The classical control scheme of a conventional binary distillation column can be represented by

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} 1 & D_{12} \\ D_{21} & 1 \end{bmatrix} \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix} \begin{bmatrix} x_D^s - x_D \\ x_B^s - x_B \end{bmatrix} \tag{1}$$

After substituting the design conditions for the decouplers, Equation 1 becomes

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} M_{11} - \dfrac{M_{12}M_{21}}{M_{22}} & 0 \\ 0 & M_{22} - \dfrac{M_{12}M_{21}}{M_{11}} \end{bmatrix} \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix} \begin{bmatrix} x_D^s - x_D \\ x_B^s - x_B \end{bmatrix} \tag{2}$$

Equation 2 (the values of M's are given in Table 5) is used to plot the Bode diagrams (Figures 1-4) from which the cross over frequency (ω_{co}) and ultimate gain (K_u) were obtained. Finally, Zeigler-Nichols settings were used to obtain the feedback controller specifications, which are listed in Table 1.

Modified Column, Case I - Reflux rate and main boil-up rate are used as the feedback control variables. The design equations for the feedback control scheme are

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \bar{M}_{11} & \bar{M}_{12} \\ \bar{M}_{21} & \bar{M}_{22} \end{bmatrix} \begin{bmatrix} 1 & \bar{D}_{12} \\ \bar{D}_{21} & 1 \end{bmatrix} \begin{bmatrix} \bar{B}_1 & 0 \\ 0 & \bar{B}_2 \end{bmatrix} \begin{bmatrix} x_D^s - x_D \\ x_B^s - x_B \end{bmatrix} \tag{3}$$

and

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \bar{M}_{11} - \dfrac{\bar{M}_{12}\bar{M}_{21}}{M_{22}} & 0 \\ 0 & \bar{M}_{22} - \dfrac{\bar{M}_{11}\bar{M}_{21}}{\bar{M}_{11}} \end{bmatrix} \begin{bmatrix} \bar{B}_1 & 0 \\ 0 & \bar{B}_2 \end{bmatrix} \begin{bmatrix} x_D^s - x_D \\ x_B^s - x_B \end{bmatrix} \tag{4}$$

Equation 4 is used to plot the Bode diagrams (Figs. 1-4), and the feedback controller settings are obtained in as explained in the previous case and are listed in Table 1.

Modified Column, Case II - Here, intermediate heat exchanger duties are used as the feedback control variables. The necessary design equations are

$$\begin{bmatrix} x_c \\ x_b \end{bmatrix} = \begin{bmatrix} \bar{M}_{11} & \bar{M}_{12} \\ \bar{M}_{21} & \bar{M}_{22} \end{bmatrix} \begin{bmatrix} 1 & \bar{D}_{12} \\ \bar{D}_{21} & 1 \end{bmatrix} \begin{bmatrix} \bar{B}_1 & 0 \\ 0 & \bar{B}_2 \end{bmatrix} \begin{bmatrix} x_c^s - x_c \\ x_b^s - x_b \end{bmatrix} \tag{5}$$

and

$$\begin{bmatrix} x_c \\ \\ x_b \end{bmatrix} = \begin{bmatrix} \bar{M}_{11} - \dfrac{\bar{M}_{11}\bar{M}_{21}}{\bar{M}_{22}} & 0 \\ \\ 0 & \bar{M}_{22} - \dfrac{\bar{M}_{11}\bar{M}_{21}}{\bar{M}_{11}} \end{bmatrix} \begin{bmatrix} \bar{B}_1 & 0 \\ \\ 0 & \bar{B}_2 \end{bmatrix} \begin{bmatrix} x_c^s - x_c \\ \\ x_b^s - x_b \end{bmatrix} \qquad (6)$$

Bode diagrams are plotted using Equations 6 (Figs. 1-4) and corresponding controller settings are listed in Table 1.

Table 1. ZEIGLER-NICHOLS SETTINGS FOR THE FEEDBACK CONTROLLERS

	Conventional Column		Modified Column Case I		Modified Column Case II	
	x_D	x_B	x_D	x_B	x_c	x_b
ω_{co}	0.17	0.18	0.18	0.19	0.23	0.21
K_u	980	-850	460	-480	130	-110
$K_c = 0.45\ K_u$	415	-380	210	-215	60	-50
$\tau_I = 2\pi/1.2\omega_{co}$	30	29	29	28	23	25

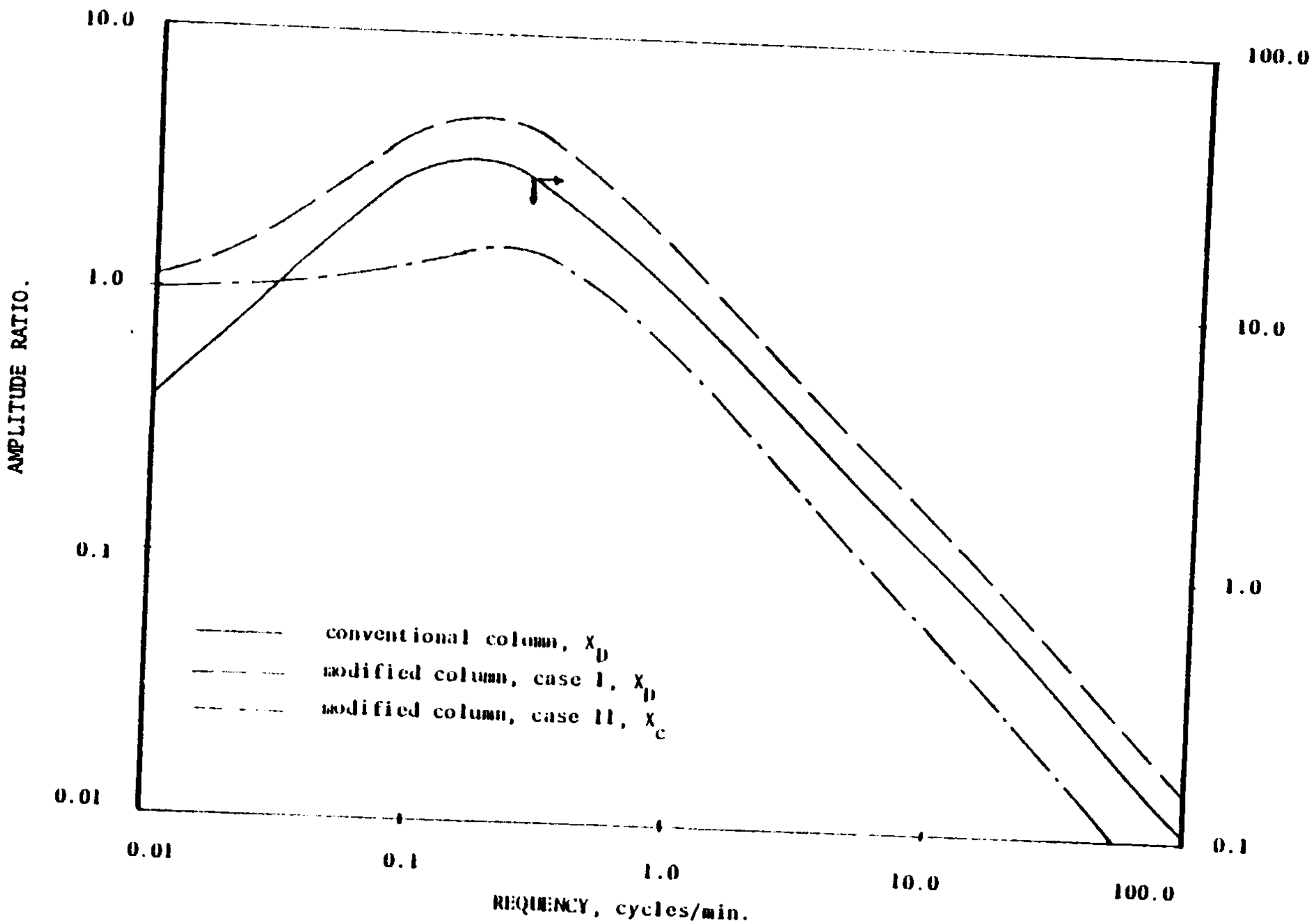

Figure 1. Bode diagram representing amplitude ratio.

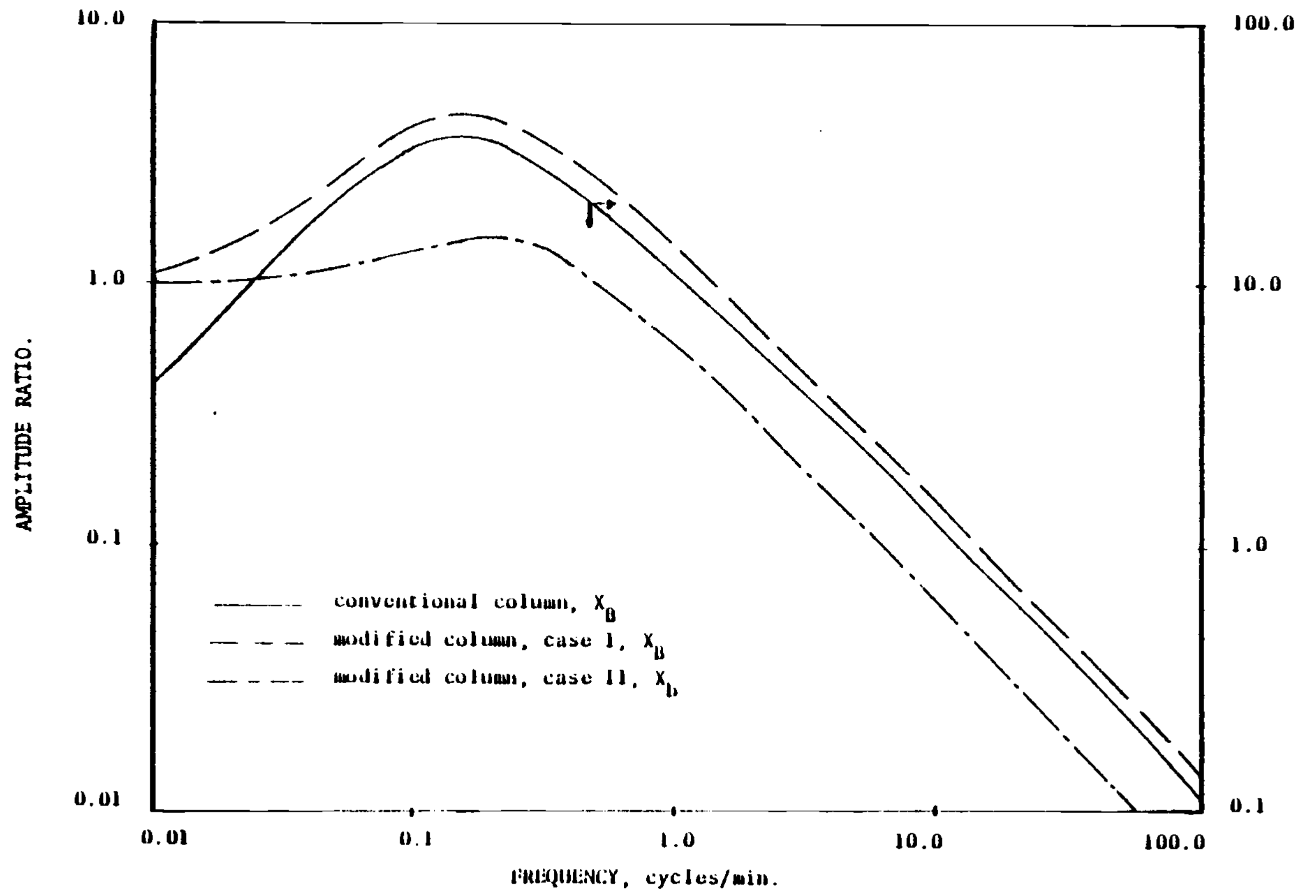

Figure 2. Bode diagram representing amplitude ratio.

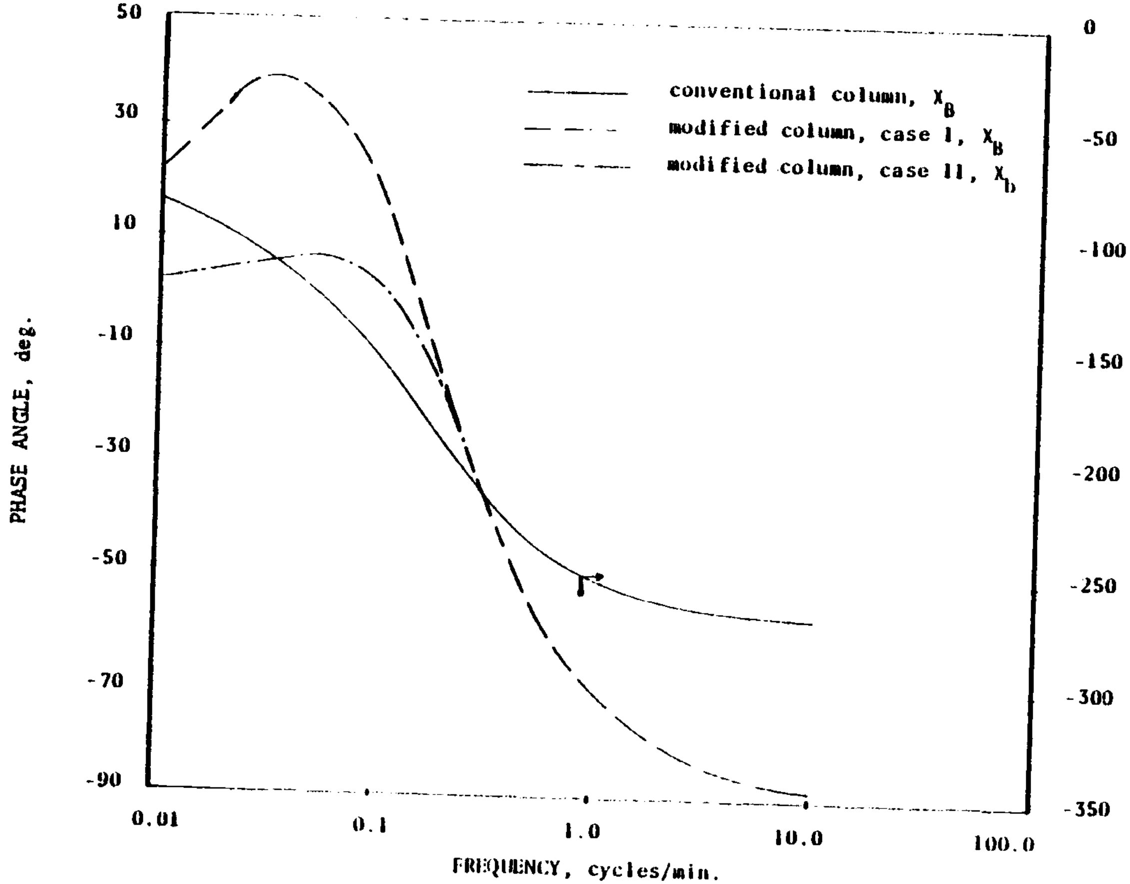

Figure 3. Bode diagram representing phase angle.

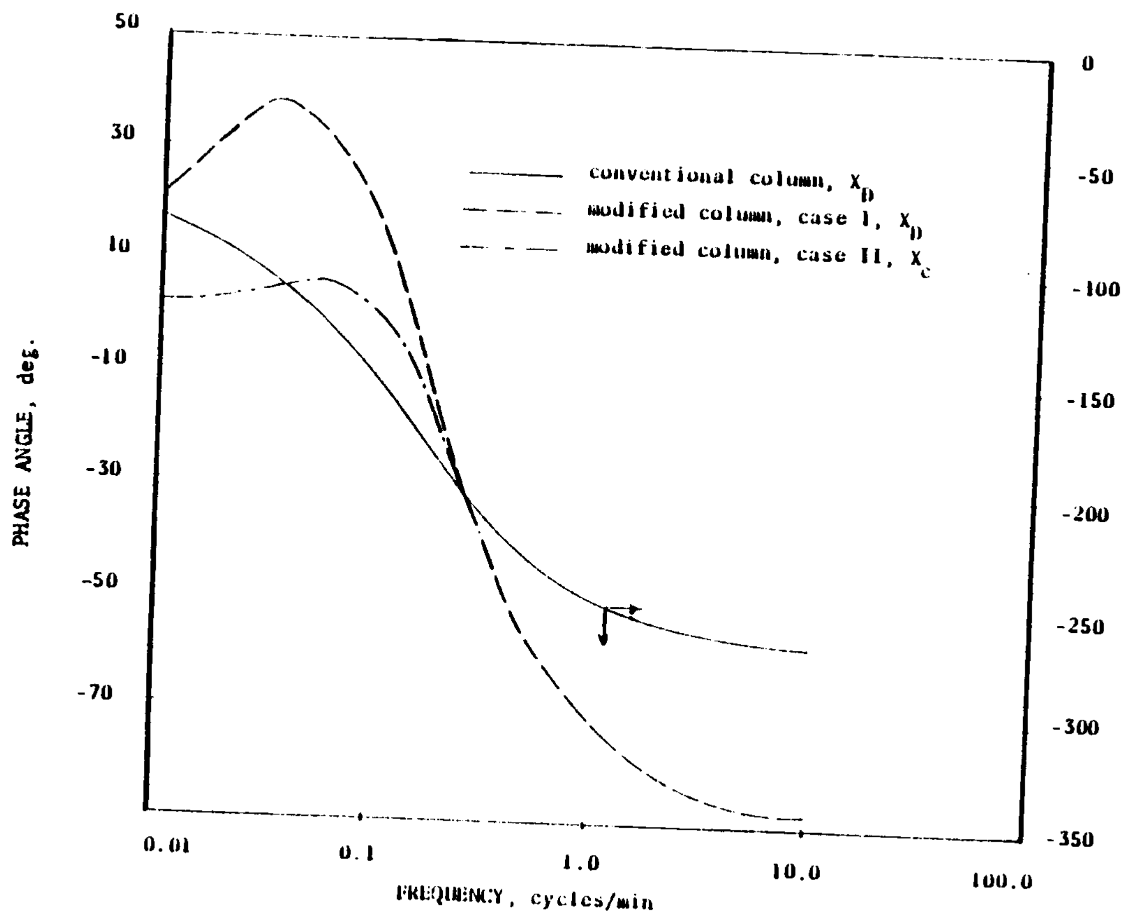

Figure 4. Bode diagram representing phase angle.

APPENDIX D

Case I: Feedforward through U - The design requirement for the feedforward control from Equation 26 is

$$F_{II} = -\bar{M}_{II}^{-1} P_I.$$

The necessary elements of the matrices M and P are given in Table 6. After going through the necessary algebraic manipulations to get the inverse of matrix of $\bar{M}_{II}$, let

$$\bar{M}_{II}^{-1} = \begin{pmatrix} M_1 & M_2 \\ M_3 & M_4 \end{pmatrix}$$

where

$$M_1 = \frac{8.5987(4.8010s+1)(5.6159s+1)(7.2773s+1)}{(s+0.01648)(s+0.07234)}$$

$$M_2 = \frac{-5.7794(4.8010s+1)(6.5944s+1)(7.2773s+1)}{(s+0.01648)(s+0.07274)}$$

$$M_3 = \frac{7.9166(4.8010s+1)(5.6159s+1)(6.5944s+1)}{(s+0.01648)(s+0.07234)}$$

$$M_4 = \frac{-6.4723(5.6159s+1)(6.5944s+1)(7.2773s+1)}{(s+0.01648)(s+0.07274)}$$

By multiplying $\bar{M}_{II}^{-1}$ and P_I, we get the feedforward matrix in the Laplace domain. By applying the partial fraction method and taking Laplace inverses, the necessary time domain equations are obtained. Therefore

$$F_{11} = 0.4964 - 1.7231\ e^{-0.165t} - 1.1137\ e^{-0.0727t}$$

$$+ 4.3424\ e^{-1.003t} - 447.5\ e^{-0.557t}$$

$$+ 444.0\ e^{-0.533t} + 3.1376\ e^{-0.0513t}$$

$$F_{21} = 0.9875 - 1.096\ e^{-0.165t} - 1.9546\ e^{-0.0727t}$$

$$+ 0.3218\ e^{-1.003t} - 299.9\ e^{-0.5575}$$

$$+ 299.7\ e^{-0.533t} + 3.4178\ e^{-0.0513t}$$

These two equations give the appropriate corrective actions on the intermediate condenser and/or reboiler in case of disturbance in feed rate.

Case II: Feedforward through U - The necessary design requirement for this case from Equation 28 is

$$F_I = -\bar{M}_I^{-1} P_I$$

Again the elements of the matrices M and P are given in Table 7. Similar algebraic manipulations as in Case I are computed to obtain the time domain feedforward design equations. Therefore

$$F_{11} = 4.4038 - 0.0196\ e^{-0.179t} - 0.9992\ e^{-0.0182t}$$

$$+ 179.5\ e^{-0.534t} - 180.2\ e^{-0.537t}$$

$$- 1.9766\ e^{-0.0513t} + 0.1484\ e^{-1.003t}$$

$$F_{21} = 5.4093 - 0.0210\, e^{-0.179t} - 1.1803\, e^{-0.0182t} + 296.8\, e^{-0.534t} - 297.6\, e^{-0.537t} - 2.303\, e^{-0.0513t} + 0.1179\, e^{-1.003t}$$

These equations give necessary corrective action on the reflux rate and/or main boil-up rates, in case of disturbance in feed rate.

APPENDIX E

1. DISTNLM -- This program is used to simulate the dynamic behavior of the distillation column(both conventional and modified). The same program can be used to obtain the initial steady state compositions as well as the steady state gains by choosing/changing the appropriate command statements.

```
      PROGRAM DISTNLM(INPUT,OUTPUT,TAPE5,TAPE6=OUTPUT,TAPE7)
      REAL LPP,LP,LB,LBB
      EXTERNAL FCN1
      DIMENSION DX(50),C(24),W(50,12),XA(50),X1(50)
      COMMON/STG/JF,JIB,JIC
      COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1           DSL,DSV,DF,DZ,B,FL(50),SV,SL
      COMMON/VAR/H0,H,F,Z,X(50),Y(50),Q,ALPA
      DATA (X1(I),I=1,20)/.0454,.0766,.1183,.1705,.2304,.2930,.3523,
     1                    .4032,.4436,.4737,.4979,.5186,.5497,.5891,
     2                    .6368,.6913,.7501,.8093,.8649,.9141/
C
C     SPECIFY THE COLUMN PARAMETERS
C
      H0=100.
      H=10.
      F=100.
      D=50.
      R=2.04
      ALPA=2.
      RMR=1.2
      Q=1.
      Z=0.5
      SV=35.146
      SL=35.146
      LBB=R*D-SL
      VPP=D*(R+1.)-SV
      VP=VPP+SV
      VB=VP+(1.-Q)*F
      VBB=VB-SL
      LB=LBB+SL
      LP=LB+Q*F
      LPP=LP-SV
      B=LPP-VPP
      DA=VBB-LBB
      DLBB=0.1*LBB
      DVPP=0.
      DSL=0.
      DSV=0.
      DF=0.
      DZ=0.
```

```
C
C     SPECIFY THE TOTAL NO. OF STAGES, FEED STAGE, INTERSTAGE
C     REBOILER AND CONDENSOR STAGE NUMBERS
C
      N=20
      JF=11
      JIB=6
      JIC=16
C
C     IF YOU WANT THE INITIAL STEADY STATE COMPOSITIONS AT EACH
C     STAGE, SET ISTD=0, IF NOT SET ISTD=1
C
      ISTD=1
      IF(ISTD.EQ.1) GO TO 20
      DO 10 I=1,N
   10 X1(I)=0.
      CALL SSNLM(N,X1)
      WRITE(6,15)
   15 FORMAT(//10X,*THE INITIAL STEADY STATE STAGE CONCNS.*,//)
      WRITE(6,25)(X1(I),I=1,N)
   25 FORMAT(5(2X,F5.4))
   20 XD=YEQLM(X1(N))
C
C     PRINT OUT THE INITIAL STEADYSTATE CONDITIONS DESCRIBING THE
C     WHOLE COLUMN
C
      CALL CISSC(X1(1),XD,DA,R,RMR,N)
C
C     PRINT THE CHANGES IN LOAD
C
      CALL CHLOAD(DF,DZ,DLBB,DVPP,DSL,DSV)
      TEND=0.
      WRITE(6,30)
   30 FORMAT(///10X,*TIME(MIN)*,6X,*XB*,5X,*XIB*,4X,*XF*,5X,
     1       *XIC*,4X,*XD*,//)
      WRITE(6,40)TEND,X1(1),X1(JIB),X1(JF),X1(JIC),XD
      WRITE(7,40)TEND,X1(1),X1(JIB),X1(JF),X1(JIC),XD
   40 FORMAT(10X,F6.3,6X,5(2X,F5.4))
      NW=50
      TOL=0.0001
      IND=1
      T=0.
      TEND=0.3
C
C     SET THE COLUMN PARAMETERS TO NEW STEADY STATE CONDITIONS.
C
   80 LBB=LBB+DLBB
      VPP=VPP+DVPP
      SL=SL+DSL
      SV=SV+DSV
```

```
      Z=Z+DZ
      F=F+DF
      LB=LBB+SL
      LP=LB+Q*F
      LPP=LP-SV
      VP=VPP+SV
      VB=VP+(1.-Q)*F
      VBB=VB-SL
      DA=VBB-LBB
      B=LPP-VPP
      R=LBB/DA
      DO 60 L=1,10
      CALL DVERK(N,FCN1,T,X1,TEND,TOL,IND,C,NW,W,IER)
      WRITE(6,40)TEND,X1(1),X1(JIB),X1(JF),X1(JIC),Y(N)
      WRITE(7,40)TEND,X1(1),X1(JIB),X1(JF),X1(JIC),Y(N)
      T=TEND
60    TEND=TEND+0.3
      IF(T.GE.6.0) GO TO 70
      DF=-2.*DF
      DZ=-2.*DZ
      DLBB=-2.*DLBB
      DVPP=-2.*DVPP
      DSV=-2.*DSV
      DSL=-2.*DSL
      GO TO 80
70    DF=-.5*DF
      DZ=-.5*DZ
      DLBB=-.5*DLBB
      DVPP=-.5*DVPP
      DSV=-.5*DSV
      DSL=-.5*DSL
      LBB=LBB+DLBB
      VPP=VPP+DVPP
      SL=SL+DSL
      SV=SV+DSV
      Z=Z+DZ
      F=F+DF
      LB=LBB+SL
      LP=LB+Q*F
      LPP=LP-SV
      VP=VPP+SV
      VB=VP+(1.-Q)*F
      VBB=VB-SL
      DA=VBB-LBB
      B=LPP-VPP
      R=LBB/DA
      TEND=6.2
      DO 90 M=1,30
      CALL DVERK(N,FCN1,T,X1,TEND,TOL,IND,C,NW,W,IER)
```

```
      WRITE(6,40)TEND,X1(1),X1(JIB),X1(JF),X1(JIC),Y(N)
      WRITE(7,40)TEND,X1(1),X1(JIB),X1(JF),X1(JIC),Y(N)
      T=TEND
   90 TEND=TEND+0.2
C
C     PRINT THE NEW STEADY STATE CONDITIONS
C
      WRITE(6,50)
   50 FORMAT(///10X,*THE NEW STEADY STATE CONDITIONS ARE*)
      CALL CISSC(X1(1),Y(N),DA,R,RMR,N)
      STOP
      END
C
C     THIS SUBROUTINE PRINTS THE CHANGE IN LOAD
C
      SUBROUTINE CHLOAD(A,B,C,D,E,F)
      WRITE(6,10)A,B,C,D,E,F
   10 FORMAT(///10X,*THE CHANGES IN LOAD ARE*,/10X,*DF     =*,F7.3,
     1       /10X,*DZ     =*,F7.3,/10X,*DLBB  =*,F7.3,
     2       /10X,*DVPP   =*,F7.3,/10X,*DSL   =*,F7.3,
     3       /10X,*DSV    =*,F7.3)
      RETURN
      END
C
C     THIS SUBROUTINE DESCRIBES THE INITIAL STEADY STATE
C     CONDITIONS OF THE COLUMN
C
      SUBROUTINE CISSC(XB,XD,DA,R,RMR,N)
      COMMON/STG/JF,JIB,JIC
      COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1           DSL,DSV,DF,DZ,B,FL(50),SV,SL
      COMMON/VAR/HO,H,F,Z,X(50),Y(50),Q,ALPA
      WRITE(6,10)ALPA,N,JF,JIB,JIC
   10 FORMAT(///10X,*RELATIVE VOLATILITY*,21X,F7.3,/10X,
     1       *NUMBER OF PLATES*,22X,I5,/10X,
     2       *FEED PLATE(FROM BOTTOM)*,15X,I5,/10X,
     3       *INTERMEDIATE REBOILER PLATE*,11X,I5,/10X,
     4       *INTERMEDIATE CONDENSOR PLATE*,10X,I5)
      WRITE(6,20)Z,XD,XB
   20 FORMAT(/10X,*FEED COMPOSITION*,24X,F7.3,/10X,
     1       *TOP PRODUCT COMPOSITION*,17X,F7.3,/10X,
     2       *BOTTOMS PRODUCT COMPOSITION*,13X,F7.3)
      WRITE(6,30)F,DA,B,LBB,VPP,SV,SL
   30 FORMAT(/10X,*FEED RATE, MOLES/MIN*,20X,F7.3,/10X,
     1       *DISTILLATE RATE, MOLES/MIN*,14X,F7.3,/10X,
     2       *BOTTOMS PRODUCT RATE, MOLES/MIN*,9X,F7.3,/10X,
     3       *REFLUX RATE, MOLES/MIN*,18X,F7.3,/10X,
     4       *MAIN BOIL-UP RATE, MOLES/MIN*,12X,F7.3,/10X,
     5       *INTERM. BOIL-UP RATE, MOLES/MIN*,9X,F7.3,/10X,
     6       *INTERM. COND. LOAD, MOLES/MIN*,11X,F7.3)
```

```
      WRITE(6,40)R,RMR,H,H0
   40 FORMAT(/10X,*REFLUX RATIO*,28X,F7.3,/10X,
     1       *REFLUX/MINIMUM REFLUX*,19X,F7.3,/10X,
     2       *PLATE HOLD UP, MOLES/PLATE*,14X,F7.3,/10X,
     3       *REBOILER HOLD UP, MOLES*,17X,F7.3)
      RETURN
      END
C
C     THIS SUBROUTINE DESCRIBES THE DIFFERENTIAL EQUATIONS
C     FOR THE NON-LINEAR MODEL
C
      SUBROUTINE FCN1(N,T,X1,XP)
      REAL LPP,LP,LB,LBB
      COMMON/STG/JF,JIB,JIC
      COMMON/VAR/H0,H,F,Z,X(50),Y(50),Q,ALPA
      COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1           DSL,DSV,DF,DZ,B,FL(50),SV,SL
      DIMENSION X1(50),XP(50)
      DO 10 I=1,N
   10 Y(I)=YEQLM(X1(I))
      XP(1)=(-VPP*Y(1)+LPP*X1(2)-B*X1(1))/H0
      JJ=JIB-1
      DO 20 J=2,JJ
   20 XP(J)=(VPP*(Y(J-1)-Y(J))+LPP*(X1(J+1)-X1(J)))/H
      XP(JIB)=(VPP*Y(JJ)-VP*Y(JIB)+LP*X1(JIB+1)-LPP*X1(JIB))/H
      JK=JIB+1
      JL=JF-1
      DO 30 K=JK,JL
   30 XP(K)=(VP*(Y(K-1)-Y(K))+LP*(X1(K+1)-X1(K)))/H
      XP(JF)=(VP*Y(JL)-VB*Y(JF)+LB*X1(JF+1)-LP*X1(JF)+F*Z)/H
      JM=JF+1
      JN=JIC-1
      DO 40 L=JM,JN
   40 XP(L)=(VB*(Y(L-1)-Y(L))+LB*(X1(L+1)-X1(L)))/H
      XP(JIC)=(VB*Y(JN)-VBB*Y(JIC)+LBB*X1(JIC+1)-LB*X1(JIC))/H
      JP=JIC+1
      JQ=N-1
      DO 50 M=JP,JQ
   50 XP(M)=(VBB*(Y(M-1)-Y(M))+LBB*(X1(M+1)-X1(M)))/H
      XP(N)=(VBB*(Y(N-1)-Y(N))+LBB*(Y(N)-X1(N)))/H
      RETURN
      END
```

```
C
C      THIS SBROUTINE EVALUATES THE INITIAL STEADY STATE CONCNS.
C      AT EACH STAGE USING NONLINEAR MODEL
C
       SUBROUTINE SSNLM(N,X1)
       EXTERNAL FCN1
       COMMON/STG/JF,JIB,JIC
       COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1            DSL,DSV,DF,DZ,B,FL(50),SV,SL
       COMMON/VAR/H0,H,F,Z,X(50),Y(50),Q,ALPA
       DIMENSION C(24),W(50,12),X1(50)
C      INITIALIZE THE STAGE CONCNS.
       XINC=1./FLOAT(N+1)
       X1(1)=XINC
       DO 10 I=2,N
   10  X1(I)=X(I-1)+XINC
C      SPECIFY THE CONDITIONS FOR THE SUBROUTINE DVERK AND SOLVE
C      THE DIFFERENTIAL EQUATIONS
       NW=50
       TOL=0.0001
       IND=1
       T=0.
       TEND=.3
       DO 20 J=1,7
       CALL DVERK(N,FCN1,T,X1,TEND,TOL,IND,C,NW,W,IER)
       T=TEND
       TEND=TEND+.3
   20  CONTINUE
       RETURN
       END
C
C      THIS FUNCTION EVALUATES THE EQUILLIBRIUM VAPOUR CONCNS.
C
       FUNCTION YEQLM(X3)
       COMMON/VAR/H0,H,F,Z,X(50),Y(50),Q,ALPA
       YEQLM=ALPA*X3/(1.+(ALPA-1.)*X3)
       RETURN
       END
 EOI ENCOUNTERED.
/
```

2. FITNLMR -- This program is used for curve fitting the dynamic response of the distillation columns. Dynamic response data is read from a stored file and the output gives the time constant(s) for the best fit of the curve.

```
      PROGRAM FITNLMR(INPUT,OUTPUT,TAPE5,TAPE6=OUTPUT)
      EXTERNAL FCN
      DIMENSION PARM(4),X(3),F(51),XJAC(51,3),XJTJ(6),WORK(123)
      DIMENSION Y1(51),Y2(51),Y3(51),Y4(51)
      COMMON/VAR/YN(51),V(51),ST1,ST2,T2,T3
      ST1=10.
      ST2=20.
      YSS=0.6956
      FK=0.013129
      FA=3.515
      ISHIFT=0
      N=1
      T2=0.
      T3=0.
      M=51
      IXJAC=51
      NSIG=3
      EPS=0.
      DELTA=0.
      IOPT=1
      MAXFN=500
      X(1)=1.
      READ(5,10)(V(I),Y1(I),Y2(I),Y3(I),Y4(I),I=1,M)
10    FORMAT(10X,F6.3,8X,F5.4,2X,F5.4,9X,F5.4,2X,F5.4)
      M=M-ISHIFT
      DO 15 I=1,M
      V(I)=V(I+ISHIFT)
15    Y3(I)=Y3(I+ISHIFT)
      CALL YNORM(M,FK,FA,YSS,Y3,YN)
      CALL ZXSSQ(FCN,M,N,NSIG,EPS,DELTA,MAXFN,IOPT,PARM,X,SSQ,
     1           F,XJAC,IXJAC,XJTJ,WORK,INFER,IER)
      WRITE(6,20)(X(I),I=1,N),SSQ
20    FORMAT(///5X,*T1 T2 & T3 ARE    *,E15.5,//5X,
     1       *SSQ            =  *,F10.6)
      WRITE(6,25)T2,T3
25    FORMAT(//2X,2E14.4)
      WRITE(6,30)(WORK(I),I=1,5),INFER,IER
30    FORMAT(//5X,*NORM OF GRAD.              =  *,E9.3,
     1          /5X,*FUNCTION EVALUATIONS     =  *,F6.1,
     2          /5X,*SIGN. DIGITS IN X        =  *,F4.1,
     3          /5X,*MARQUARDT PARAMETR       =  *,E9.3,
     4          /5X,*NO. OF ITERATIONS        =  *,F6.1,
     5          /5X,*CRITERIAN                =  *,I2,
     6          /5X,*IER                      =  *,I5)
      STOP
      END
```

```
C
C
C THIS SUBROUTINE DESCRIBES THE RESPONSE FUNCTION TO BE FIT
C
C
      SUBROUTINE FCN(X,M,N,F)
      DIMENSION X(N),F(M),Y1(51),XX(3)
      COMMON/VAR/YN(51),V(51),ST1,ST2,T2,T3
      DO 5 I=1,N
      XX(I)=X(I)
      IF(XX(I).LT.0.1) XX(I)=0.1
  5   CONTINUE
      T1=XX(1)
      IF(N.EQ.1) GO TO 10
      T2=XX(2)
      IF(N.EQ.2) GO TO 10
      T3=XX(3)
 10   T13=T1-T3
      T32=T3-T2
      T21=T2-T1
      IF(ABS(T21).LT.1.0E-10) T21=SIGN(T21,1.0E-10)
      DO 20 I=1,10
 20   Y1(I)=1.+T13*EXP(-V(I)/T1)/T21
      IF(N.EQ.1) GO TO 40
      DO 30 I=1,10
 30   Y1(I)=Y1(I)+T32*EXP(-V(I)/T2)/T21
 40   DO 50 I=11,20
 50   Y1(I)=-1.+(T13/T21)*(EXP(-V(I)/T1)-2.*EXP((ST1-V(I))/T1))
      IF(N.EQ.1) GO TO 70
      DO 60 I=11,20
 60   Y1(I)=Y1(I)+(T32/T21)*(EXP(-V(I)/T2)-2.*EXP((ST1-V(I))/T2))
 70   DO 80 I=21,M
 80   Y1(I)=(T13/T21)*(EXP(-V(I)/T1)-2.*EXP((ST1-V(I))/T1)+
     1          EXP((ST2-V(I))/T1))
      IF(N.EQ.1) GO TO 100
      DO 90 I=21,M
 90   Y1(I)=Y1(I)+(T32/T21)*(EXP(-V(I)/T2)-2.*EXP((ST1-V(I))/T2)
     1                +EXP((ST2-V(I))/T2))
100   DO 110 I=1,M
110   F(I)=YN(I)-Y1(I)
      RETURN
      END
C
C THIS SUBROUTINE NORMALILZES THE DATA PONTS
C
      SUBROUTINE YNORM(M,FK,FA,YSS,Y,YN)
      DIMENSION Y(M),YN(M)
      DO 10 I=1,M
 10   YN(I)=(Y(I)-YSS)/FK/FA
      RETURN
      END
 EOI ENCOUNTERED.
/
```

3. FFCNTR -- This program is used to simulate the control response of the distillation column - case I. The same program can be used to simulate the control response of the conventional and modified columns without feedforward correction, by removing the feedforward correction commands.

```
      PROGRAM FFCNTR(INPUT,OUTPUT,TAPE5,TAPE6=OUTPUT,TAPE7)
      COMMON/CSETT/DK.BK.TID.TIB
      COMMON/DSETT/A1,B1.A2.B2
      COMMON/TIME/DT
      COMMON/SDSTG/X2(50)
      DIMENSION X(50)
      REAL LBB
      DATA (X2(I),I=1,20)/.0538,.0876,.1289..1760..2258,.2741,.3371,
     1                    .3928,.4378,.4716,.4956,.5239..5609..6072.
     2                    .6622,.7237,.7602,.8023..8487,.8974/
C
C     SPECIFY THE INITIAL PARAMETERS & DISTUBANCCE
C
      T1=0.
      XF=100.
      XZ=0.5
      DF=10.0
      DZ=0.0
      XF=XF+DF
      XZ=XZ+DZ
      D=50.
      R=2.04
      XSL=35.146
      XSV=35.146
      XLBB=R*D-XSL
      XVPP=D*(R+1.)-XSV
      XDS=0.0
      XBS=0.0
C
C     SET THE INITIAL CONTROLLER & DECOUPLER OUTPUT TO ZERO
C
      CD0=0.
      CB0=0.
      CDB0=0.
      CBB0=0.
      ED0=0.
      EB0=0.
```

```
C
C     SOLVE THE NONLINEAR MODEL TO GET NEW XD & XB DUE TO CHANE IN Z/F
C
      DT=.1
      DO 5 I=1,20
    5 X(I)=X2(I)
      CALL PRDYNM(XF,XZ,XSL,XSV.XLBB,XVPP,X,T1,XD,XB)
      WRITE(6,10)T1,XZ,XLBB,XVPP,ED0,EB0,CD0,CB0,CDB0.CBB0,XD,XB
   10 FORMAT(12(2X,F8.4))
      WRITE(7,30)T1,XD,XB,XLBB.XVPP,XSL,XSV
   30 FORMAT(F4.1,1X,F6.4,1X,F6.4.4(1X.F8.4))
C
C     CHANGE THE TIME REFERENCE AND CALCULATE THE ERROR
C
      K=1
      T1=T1+DT
      SUMED=0.
      SUMEB=0.
      ED=XDS-XD
      EB=XBS-XB
      SUMED=SUMED+ED
      SUMEB=SUMEB+EB
C
C     SPECIFY THE CONTROLLER SETTINGS & EVALUATE THE CONTROLLER OUTPUT
C
      DK=2500.0
      TID=1.0
      BK=-2500.0
      TIB=1.0
      CALL CONTOUT(K,ED,EB,SUMED,SUMEB,CD1,CB1)
C
C     GET THE FEED FORWARD CRRECTION FOR SL & SV
C
      CALL FRWCONT(T1,F11,F21,F12,F22)
      XSL=35.146+F11*DF+F12*DZ
      XSV=35.146+F21*DF+F22*DZ
      DO 25 II=1,20
   25 X(II)=X2(II)
      CALL PRDYNM(XF,XZ,XSL,XSV,XLBB,XVPP,X,T1,XD,XB)
      WRITE(6,10)T1,XZ.XLBB,XVPP,ED,EB,CD1,CB1,CDB0,CBB0,XD,XB
      WRITE(7,30)T1,XD,XB,XLBB,XVPP,XSL,XSV
      K=2
      T1=T1+DT
   20 ED=XDS-XD
      EB=XBS-XB
      IF(K.GE.100) STOP
      SUMED=SUMED+ED
      SUMEB=SUMEB+EB
      CALL CONTOUT(K,ED,EB,SUMED,SUMEB,CD,CB)
```

```
C
C      SPECIFY THE DECOUPLER SETTINGS & EVALUATE DECOUPLER OUTPT
C
       A1=5.2739
       A2=4.5703
       B1=6.6443
       B2=5.8698
       CALL DECPOUT(CD1,CB1,CDB0,CBB0,CD,CB,CDB,CBB)
       CD1=CD
       CB1=CB
       CDB0=CDB
       CBB0=CBB
C
C      MAKE CORRECTIVE CHANGES IN L & V
C
       XLBB=66.854+(CD+CBB)
       XVPP=116.854+(CB+CDB)
C
C      GET THE FEED FORWARD CORRECTION FOR SL & SV
C
       CALL FRWCONT(T1,F11,F21,F12,F22)
       XSL=35.146+F11*DF+F12*DZ
       XSV=35.146+F21*DF+F22*DZ
C
C      SOLVE THE NONLINEAR DYNAMICS WITH NEW VARIABLES
C
       DO 15 J=1,20
  15   X(J)=X2(J)
       CALL PRDYNM(XF,XZ,XSL,XSV,XLBB,XVPP,X,T1,XD,XB)
       WRITE(6,10)T1,XZ,XLBB,XVPP,ED,EB,CD,CB,CDB,CBB,XD,XB
       WRITE(7,30)T1,XD,XB,XLBB,XVPP,XSL,XSV
       K=K+1
       T1=T1+DT
       GO TO 20
       STOP
       END
C
C
C      THIS SUBROUTINE EVALUATES CONTROLLER OUTPUT
C
C
       SUBROUTINE CONTOUT(K,ED,EB,SUMED,SUMEB,CD,CB)
       COMMON/CSETT/DK,BK,TID,TIB
       COMMON/TIME/DT
       CD=DK*(ED+DT/TID*SUMED)
       CB=BK*(EB+DT/TIB*SUMEB)
       RETURN
       END
```

```
C
C     THIS SUBROUTINE EVALUATES DECOUPLE OUTPUT
C
      SUBROUTINE DECPOUT(CD0,CB0,CDB0,CBB0,CD,CB,CDB,CBB)
      COMMON/DSETT/A1,B1,A2,B2
      COMMON/TIME/DT
      CDB=CDB0+DT/B1*((1.0606*CD-CDB0)+1.0606*A1/DT*(CD-CD0))
      CBB=CBB0+DT/B2*((.8938*CB-CBB0)+.8938*A2/DT*(CB-CB0))
      RETURN
      END
C
C     THIS SUBROUTINE EVALUATES THE FEED FORWARD CORRECTIONS
C
      SUBROUTINE FRWCONT(T,F11,F21,F12,F22)
      F11=0.4964-1.7231*EXP(-.16483*T)-1.1137*EXP(-.07274*T)
     1          +4.3424*EXP(-1.0030*T)-447.4956*EXP(-.5373*T)
     2          +444.0019*EXP(-.5327*T)+3.1376*EXP(-.05132*T)
      F21=0.9875-1.096*EXP(-.16483*T)-1.9546*EXP(-.07274*T)
     1          +0.3218*EXP(-1.003*T)-299.8812*EXP(-.5373*T)
     2          +299.6963*EXP(-.5327*T)+3.4178*EXP(-.05132*T)
      F12=-86.23-277.023*EXP(-.16483*T)+147.4505*EXP(-.07274*T)
     1          +1120.8292*EXP(-.8128*T)-1395.5837*EXP(-.7329*T)
     2          +982.5786*EXP(-.2426*T)-599.6215*EXP(.2303*T)
      F22=28.1-294.4583*EXP(-.16483*T)+152.7341*EXP(-.07274*T)
     1        +1110.891*EXP(-.8128*T)-1630.2621*EXP(-.7329*T)
     2        +1193.984*EXP(-.2426*T)-701.9131*EXP(-.2303*T)
      RETURN
      END
C
C     THIS SUBROUTINE SOLVES THE NONLINEAR DYNAMICS
C
      SUBROUTINE PRDYNM(XF,XZ,XSL,XSV,XLBB,XVPP,X,T1,XD,XB)
      REAL LPP,LP,LB,LBB
      EXTERNAL FCN1
      DIMENSION DX(50),C(24),W(50,12),X(50),X1(50)
      COMMON/STG/JF,JIB,JIC
      COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1           DSL,DSV,DF,DZ,B,FL(50),SV,SL
      COMMON/VAR/H0,H,F,Z,Y(50),Q,ALPA
      COMMON/TIME/DT
      COMMON/SDSTG/X2(50)
C
C     SPECIFY THE COLUMN PARAMETERS
C
      F=XF
      Z=XZ
      SL=XSL
      SV=XSV
      LBB=XLBB
      VPP=XVPP
```

```
      H0=100.
      H=10.
      D=50.
      R=2.04
      ALPA=2.
      RMR=1.2
      Q=1.
      VP=VPP+SV
      VB=VP+(1.-Q)*F
      VBB=VB-SL
      LB=LBB+SL
      LP=LB+Q*F
      LPP=LP-SV
      B=LPP-VPP
      DA=VBB-LBB
C
C     SPECIFY THE TOTAL NO. OF STAGES, FEED STAGE, INTERSTAGE
C     REBOILER AND CONDENSOR STAGE NUMBERS
C
      N=20
      JF=11
      JIB=6
      JIC=16
C
C     PRINT OUT THE INITIAL STEADYSTATE CONDITIONS DESCRIBING THE
C     WHOLE COLUMN
C
      NW=50
      TOL=0.0001
      IND=1
      T=T1
      TEND=T+DT
      DO 10 I=1,N
   10 X1(I)=X(I)
      CALL DVERK(N,FCN1,T,X1,TEND,TOL,IND,C,NW,W,IER)
      DO 20 J=1,N
   20 X2(J)=X1(J)
      XD=Y(N)-.9459
      XB=X1(1)-.0538
      RETURN
      END
C
C     THIS SUBROUTINE DESCRIBES THE DIFFERENTIAL EQUATIONS
C     FOR THE NON-LINEAR MODEL
C
      SUBROUTINE FCN1(N,T,X1,XP)
      REAL LPP,LP,LB,LBB
      COMMON/STG/JF,JIB,JIC
      COMMON/VAR/HO,H,F,Z,Y(50),Q,ALPA
```

```
      COMMON/PAR/VPP,LPP,VP.LP,VB,LB.VBB.LBB,DLBB,DVPP,
     1            DSL,DSV,DF,DZ,B.FL(50).SV,SL
      DIMENSION X1(50),XP(50)
      DO 10 I=1,N
   10 Y(I)=YEQLM(X1(I))
      XP(1)=(-VPP*Y(1)+LPP*X1(2)-B*X1(1))/HO
      JJ=JIB-1
      DO 20 J=2,JJ
   20 XP(J)=(VPP*(Y(J-1)-Y(J))+LPP*(X1(J+1)-X1(J)))/H
      XP(JIB)=(VPP*Y(JJ)-VP*Y(JIB)+LP*X1(JIB+1)-LPP*X1(JIB))/H
      JK=JIB+1
      JL=JF-1
      DO 30 K=JK,JL
   30 XP(K)=(VP*(Y(K-1)-Y(K))+LP*(X1(K+1)-X1(K)))/H
      XP(JF)=(VP*Y(JL)-VB*Y(JF)+LB*X1(JF+1)-LP*X1(JF)+F*Z)/H
      JM=JF+1
      JN=JIC-1
      DO 40 L=JM,JN
   40 XP(L)=(VB*(Y(L-1)-Y(L))+LB*(X1(L+1)-X1(L)))/H
      XP(JIC)=(VB*Y(JN)-VBB*Y(JIC)+LBB*X1(JIC+1)-LB*X1(JIC))/H
      JP=JIC+1
      JQ=N-1
      DO 50 M=JP,JQ
   50 XP(M)=(VBB*(Y(M-1)-Y(M))+LBB*(X1(M+1)-X1(M)))/H
      XP(N)=(VBB*(Y(N-1)-Y(N))+LBB*(Y(N)-X1(N)))/H
      RETURN
      END
C
C     THIS FUNCTION EVALUATES THE EQUILLIBRIUM VAPOUR CONCNS.
C
      FUNCTION YEQLM(X3)
      COMMON/VAR/HO,H,F,Z,Y(50),Q.ALPA
      YEQLM=ALPA*X3/(1.+(ALPA-1.)*X3)
      RETURN
      END
 EOI ENCOUNTERED.
/
```

Subroutines used for feedforward correction and tracking set points of case II.

```
C
C      THIS SUBROUTINE EVALUATES THE FEED FORWARD CORRECTION FOR
C      LBB & VPP
C
       SUBROUTINE FFCONT(T,F11,F21)
       F11=4.4038-.01961*EXP(-.17902*T)-.9992*EXP(-.018145*T)
     1     +179.513*EXP(-.534*T)-180.161*EXP(-.5369*T)
     2     -1.9766*EXP(-.05132*T)+.1484*EXP(-1.0029*T)
       F21=5.4093-.02095*EXP(-.17902*T)-1.1803*EXP(-.018145*T)
     1     +296.851*EXP(-.534*T)-297.567*EXP(-.5369*T)
     2     -2.303*EXP(-.05132*T)+.1179*EXP(-1.0029*T)
       RETURN
       END
C
C      THIS SUBROUTINE EVALUATES THE CHANGES IN SETPOINTS OF XIC & XIB
C
       SUBROUTINE SETPT(T,F11,F21,G11,G21)
       REAL M11,M12,M21,M22
       P11=0.008575*(1.-0.08093*(12.945*EXP(-T/12.945)-
     1                          0.58831*EXP(-T/0.58831)))
       P21=0.01426*(1.-EXP(-T/3.6452))
       M11=0.019417*(1.-EXP(-T/3.7583))
       M12=-.016235*(1.-EXP(-T/4.3793))
       M21=0.021062*(1.-EXP(-T/4.3192))
       M22=-.016680*(1.-EXP(-T/2.6817))
       G11=P11-M11*F11-M12*F21
       G21=P21-M21*F11-M22*F21
       RETURN
       END
```

4. DIST -- This subroutine is used to simulate the linear model of the distillation column.

```
      PROGRAM DIST(INPUT,OUTPUT,TAPE5,TAPE6=OUTPUT,TAPE7)
      REAL LPP,LP,LB,LBB
      EXTERNAL FCN
      DIMENSION DX(50),C(24),W(50,12),XA(50)
      COMMON/CONST/A1(7)
      COMMON/STG/JF,JIB,JIC
      COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1 DSL,DSV,DF,DZ,B,FL(50)
      COMMON/VAR/H0,H,F,Z,X(50),Y(50),Q
      COMMON/XMATX/A(20,20),B1(20,4),D1(20,2)
      DATA (X(I),I=1,15)/.1048,.1612,.2196,.2744,.342,.3997,.4444,
     1 .4766,.4986,.5287,.5705,.6261,.6956,.744,.8103/
      DATA (A1(I),I=1,7)/-0.00054249,2.02,-1.8051,1.0839,
     1     -0.29813,0.,0./
C
C     SPECIFY THE COLUMN PARAMETERS
C
      H0=2.
      H=1.25
      F=100.
      D=50.
      B=F-D
      R=1.68
      Q=1.
      Z=.5
      VPP=D*(R+1.)-35.146
      VBB=VPP
      SV=35.146
      VP=VPP+SV
      VB=VP
      SL=SV
      LBB=R*D-35.146
      LB=LBB+SL
      LPP=Q*F+LBB
      LP=LPP+SL
      DLBB=0.
      DVPP=-0.01*VPP
      DSL=0.
      DSV=-0.01*SV
      DF=0.0
      DZ=0.0
```

```
C
C      SPECIFY THE TOTAL NO. OF STAGES,FEED STAGE,INTERSTAGE REBOILER
C      AND CONDENSOR STRAGE NUMBERS
C
       N=15
       JF=9
       JIC=13
       JIB=4
C
C      SPECIFY THE INITIAL CONCN DEVIATIONS AT EACH STAGE
C
       DO 70 I=1,N
  70   DX(I)=0.
       XD=YEQLM(X(N))
C
C      IF YOU WANT TO CHECK THE SIMULATION FOR NEGATIVE DEVIATION
C      SET IBACK=0.IF NOT SET IBACK=1
C
       IBACK=1
C
C      SPECIFY THE SYSTEM TO GET THE EQUILLIBRIUM RELATION
C
       IA=4
       IF(IA.EQ.1) GO TO 125
       IF(IA.EQ.2) GO TO 135
       IF(IA.EQ.3) GO TO 145
       WRITE(6,155)
 155   FORMAT(///15X,*ETHANOL-N,PROPANOL SYSTEM*,//)
       GO TO 100
 125   WRITE(6,165)
 165   FORMAT(///15X,*BENZENE-TOLUENE SYSTEM*,//)
       GO TO 100
 135   WRITE(6,175)
 175   FORMAT(///15X,*METHANOL-WATER SYSTEM*,//)
       GO TO 100
 145   WRITE(6,185)
 185   FORMAT(///15X,*ETHANOL-I,PROPANOL SYSTEM*,//)
 100   TEND=0.
       DO 10 K=1,N
       DO 20 L=1,N
  20   A(K,L)=0.
  10   CONTINUE
       CALL AMATX(N,A)
       CALL BMATX(N,B1)
       CALL DMATX(N,D1)
       GO TO 12
  95   WRITE(6,35)
       WRITE(6,40)((A(I,J),J=1,N),I=1,N)
  35   FORMAT(///50X,*MATRIX  A*,//)
  40   FORMAT(15(F8.5))
       WRITE(6,45)
  45   FORMAT(///12X,*MATRIX  B *,40X,*MATRIX  D *,//)
       DO 60 K=1,N
       WRITE(6,50)(B1(K,M),M=1,4),(D1(K,MM),MM=1,2)
  50   FORMAT(4(1X,F8.5),20X,2(1XF8.5))
  60   CONTINUE
```

```
C
C     PRINT HEADING
C
  12  WRITE(6,195)
 195  FORMAT(///,*TIME*,6X,*XW*,5X,*X1*,5X,*X2*,5X,*X3*,5X,*X4*,5X,
     1        *X5*,5X,*X6*,5X,*X7*,5X,*X8*,5X,*X9*,5X,*X10*,4X,
     1        *X11*,4X,*X12*,4X,*X13*,4X,*X14*,4X,*XD*,/)
C
C     SPECIFY THE CONDITIONS FOR SUBRUTINE DVERK
C
      WRITE(6,80)TEND,(X(I),I=1,15),XD
      NW=50
      TOL=0.0001
      IND=1
      T=0.
      TEND=.3
      DO 75 M=1,7
      CALL DVERK(N,FCN,T,DX,TEND,TOL,IND,C,NW,W,IER)
      DO 25 IJ=1,15
  25  XA(IJ)=X(IJ)+DX(IJ)
      XDA=YEQLM(XA(N))
      WRITE(6,80)TEND,(XA(I),I=1,N),XDA
  80  FORMAT(F4.1,2X,16(2X,F5.4))
      T=TEND
      TEND=TEND+.3
  75  CONTINUE
C
C     CHECK THE SIMULATION BY GIVING NEGETIVE DEVIATION
C
      IF(IBACK.EQ.1) GO TO 90
      IBACK=IBACK+1
      LBB=LBB+DLBB
      VPP=VPP+DVPP
      SL=SL+DSL
      SV=SV+DSV
      Z=Z+DZ
      F=F+DF
      LB=LBB+SL
      LP=LB+Q*F
      LPP=LP-SV
      VP=VPP+SV
      VB=VP+(1.-Q)*F
      VBB=VB-SL
      DLBB=-DLBB
      DVPP=-DVPP
      DSL=-DSL
      DSV=-DSV
      DZ=-DZ
      DF=-DF
      DO 15 JK=1,15
  15  X(JK)=XA(JK)
      XD=XDA
      GO TO 95
  90  STOP
      END
```

```
C
C
C     THIS SUBROUTINE DESCRIBES THE DIFFERENTIAL EQUATIONS
C     TO BE SOLVED
C
C
      SUBROUTINE FCN(N,T,DX,DXP)
      COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1           DSL,DSV,DF,DZ,B,FL(50)
      COMMON/STG/JF,JIB,JIC
      COMMON/VAR/HO,H,F,Z,X(50),Y(50),Q
      COMMON/XMATX/A(20,20),B1(20,4),D1(20,2)
      DIMENSION DX(N),DXP(N)
      DXP(1)=(A(1,1)*DX(1)+A(1,2)*DX(2)+B1(1,1)*DLBB+B1(1,2)*DVPP
     1      +B1(1,3)*DSL+B1(1,4)*DSV+D1(1,1)*DF)/HO
      JJ=JIB-1
      DO 10 J=2,JJ
   10 DXP(J)=(A(J,(J-1))*DX(J-1)+A(J,J)*DX(J)+A(J,(J+1))*DX(J+1)+
     1      B1(J,1)*DLBB+B1(J,2)*DVPP+B1(J,3)*DSL+B1(J,4)*DSV
     2      +D1(J,1)*DF)/H
      DXP(JIB)=(A(JIB,JJ)*DX(JJ)+A(JIB,JIB)*DX(JIB)+A(JIB,(JIB+1))*
     1      DX(JIB+1)+B1(JIB,1)*DLBB+B1(JIB,2)*DVPP+B1(JIB,3)*DSL
     2      +B1(JIB,4)*DSV+D1(JIB,1)*DF)/H
      JK=JIB+1
      JL=JF-1
      DO 20 K=JK,JL
   20 DXP(K)=(A(K,(K-1))*DX(K-1)+A(K,K)*DX(K)+A(K,(K+1))*DX(K+1)+
     1      B1(K,1)*DLBB+B1(K,2)*DVPP+B1(K,3)*DSL+B1(K,4)*DSV+
     2      D1(K,1)*DF)/H
      DXP(JF)=(A(JF,JL)*DX(JL)+A(JF,JF)*DX(JF)+A(JF,(JF+1))*DX(JF+1)
     1      +B1(JF,1)*DLBB+B1(JF,2)*DVPP+B1(JF,3)*DSL+B1(JF,4)*DSV
     2      +D1(JF,1)*DF+D1(JF,2)*DZ)/H
      JM=JF+1
      JN=JIC-1
      DO 30 L=JM,JN
   30 DXP(L)=(A(L,(L-1))*DX(L-1)+A(L,L)*DX(L)+A(L,(L+1))*DX(L+1)
     1      +B1(L,1)*DLBB+B1(L,2)*DVPP+B1(L,3)*DSL+B1(L,4)*DSV
     2      +D1(L,1)*DF)/H
      DXP(JIC)=(A(JIC,JN)*DX(JN)+A(JIC,JIC)*DX(JIC)+A(JIC,(JIC+1))*
     1      DX(JIC+1)+B1(JIC,1)*DLBB+B1(JIC,2)*DVPP+B1(JIC,3)*DSL
     2      +B1(JIC,4)*DSV+D1(JIC,1)*DF)/H
      JP=JIC+1
      JQ=N-1
      DO 40 M=JP,JQ
   40 DXP(M)=(A(M,(M-1))*DX(M-1)+A(M,M)*DX(M)+A(M,(M+1))*DX(M+1)+
     1      B1(M,1)*DLBB+B1(M,2)*DVPP+B1(M,3)*DSL+B1(M,4)*DSV+
     2      D1(M,1)*DF)/H
      DXP(N)=(A(N,JQ)*DX(JQ)+A(N,N)*DX(N)+B1(N,1)*DLBB+B1(N,2)*DVPP+
     1      B1(N,3)*DSL+B1(N,4)*DSV+D1(N,1)*DF)/H
      RETURN
      END
C
C     THIS SUBROUTINE EVALUATES THE ELEMENTS OF MATRIX A
C
      SUBROUTINE AMATX(N,A)
      REAL LPP,LP,LB,LBB
```

```
      COMMON/STG/JF,JIB,JIC
      COMMON/PAR/VPP,LPP,VP,LP,VB,LB,VBB,LBB,DLBB,DVPP,
     1       DSL,DSV,DF,DZ,B,FL(50)
      COMMON/VAR/HO,H,F,Z,X(50),Y(50),Q
      DIMENSION A(20,20)
      DO 10 I=1,N
      Y(I)=YEQLM(X(I))
   10 FL(I)=Y(I)
      A(1,1)=-(B+VPP*FL(1))
      A(1,2)=LPP
      JJ=JIB-1
      DO 20 J=2,JJ
      J1=J-1
      J2=J+1
      A(J,J1)=VPP*FL(J1)
      A(J,J)=-VPP*FL(J)-LPP
   20 A(J,J2)=LPP
      JK=JIB+1
      JL=JF-1
      DO 30 K=JK,JL
      K1=K-1
      K2=K+1
      A(K,K1)=VP*FL(K1)
      A(K,K)=-VP*FL(K)-LP
   30 A(K,K2)=LP
      JM=JF+1
      JN=JIC-1
      DO 40 L=JM,JN
      L1=L-1
      L2=L+1
      A(L,L1)=VB*FL(L1)
      A(L,L)=-VB*FL(L)-LB
   40 A(L,L2)=LB
      JP=JIC+1
      JQ=N-1
      DO 50 M=JP,JQ
      M1=M-1
      M2=M+1
      A(M,M1)=VBB*FL(M1)
      A(M,M)=-VBB*FL(M)-LBB
   50 A(M,M2)=LBB
      A(JIB,JJ)=VPP*FL(JJ)
      A(JIB,JIB)=-VP*FL(JIB)-LPP
      A(JIB,JK)=LP
      A(JF,JL)=VP*FL(JL)
      A(JF,JF)=-VB*FL(JF)-LP
      A(JF,JM)=LB
      A(JIC,JN)=VB*FL(JN)
      A(JIC,JIC)=-VBB*FL(JIC)-LB
      A(JIC,JP)=LBB
      A(N,JQ)=VBB*FL(JQ)
      A(N,N)=-VBB*FL(N)-LBB+LBB*FL(N)
      RETURN
      END
```

```
C
C     THIS SUBROUTINE EVALUATES THE ELEMENTS OF MATRIX B
C
      SUBROUTINE BMATX(N,B)
      COMMON/STG/JF,JIB,JIC
      DIMENSION B(20,4)
      COMMON/VAR/H0,H,F,Z,X(50),Y(50),Q
      B(1,1)=(X(2)-X(1))
      B(1,2)=(X(1)-Y(1))
      B(1,3)=B(1,1)
      B(1,4)=-B(1,1)
      NN=N-1
      DO 10 I=2,NN
      B(I,1)=X(I+1)-X(I)
   10 B(I,2)=Y(I-1)-Y(I)
      JK=JIC-1
      DO 20 J=2,JK
   20 B(J,3)=X(J+1)-X(J)
      B(JIC,3)=Y(JIC)-X(JIC)
      KL=JIC+1
      DO 30 K=KL,N
   30 B(K,3)=Y(K)-Y(K-1)
      JJ=JIB-1
      DO 40 L=2,JJ
   40 B(L,4)=X(L)-X(L+1)
      B(JIB,4)=X(JIB)-Y(JIB)
      JL=JIB+1
      DO 50 M=JL,N
   50 B(M,4)=Y(M-1)-Y(M)
      B(N,1)=Y(N)-X(N)
      B(N,2)=Y(N-1)-Y(N)
      RETURN
      END
C
C     THIS SUBROUTINE EVALUATES THE ELEMENTS OF MATRIX D
C
C
      SUBROUTINE DMATX(N,D)
      COMMON/STG/JF,JIB,JIC
      COMMON/VAR/H0,H,F,Z,X(50),Y(50),Q
      DIMENSION D(20,2)
      D(1,1)=(X(2)-X(1))*Q
      D(1,2)=0.
      IJ=JF-1
      DO 10 I=2,IJ
      D(I,1)=(X(I+1)-X(I))*Q
   10 D(I,2)=0.
      D(JF,1)=Z-1.
      D(JF,2)=F
      JK=JF+1
      DO 20 J=JK,N
      D(J,2)=0.
   20 D(J,1)=(Y(J-1)-Y(J))*(1.-Q)
      RETURN
      END
```

NOMENCLATURE

B	Feedback controller matrix of the conventional column.
B_{ij}	Elements of matrix B
$\tilde{B}$	Feedback controller matrix of modified column
B_{I}	Feedback controller matrix of case I of modified column
B_{II}	Feedback controller of case II of modified column
D	Decoupler matrix of conventional column
D_{ij}	Elements of matrix D
$\tilde{D}$	Decoupler matrix of modified column
$\bar{D}_{I}$, $\bar{D}_{II}$, $\bar{\bar{D}}_{I}$, $\bar{\bar{D}}_{II}$	Partitioned matrices of $\tilde{D}$
E_r	Stage efficiency as defined in Equation 6
f	Feed rate, moles/min.
F_r	Liquid feed of composition z_r, moles/min
F_r'	Vapor feed of composition z_r', moles/min
F	Feedforward controller matrix of the modified column
F_I	Feedforward controller matrix of case I of modified column
F_{II}	Feedforward controller matrix of case II of modified column
F_{11}	Feedforward controller element for distillate rate or intermediate condenser flow
F_{21}	Feedforward controller element for main boil-up or intermediate boil-up rate
G	Set point tracking matrix

G_I	Set point tracking matrix of case I of modified column
G_{II}	Set point tracking matrix of case II of modified column
h_r	Vapor hold up above the rth stage, moles
H_0	Main boiler liquid hold up, moles
H_r	Liquid hold up on rth stage, moles
I	Identity matrix
J_r	Liquid withdrawal of composition x_r, moles/min
J'_r	Vapor withdrawal of composition y_r, moles/min
K_p	Feedback controller gain
l	Liquid flow from the intermediate condenser, moles/min
L	Reflux rate, moles/min
$\tilde{L}$	Internal liquid flow below the intermediate condenser stage and above the feed stage, moles/min
$\bar{L}$	Internal liquid flow above the intermediate condenser stage or reflux rate, moles/min
L'	Internal liquid flow below feed stage and above intermediate boiler stage, moles/min
L''	Internal liquid flow below intermediate boiler stage, moles/min
L_r	Internal liquid flow from stage r
M	Process transfer matrix of conventional column with respect to control variables
M_{ij}	Elements of matrix M
$\tilde{M}$	Process transfer matrix of modified column with respect to control variables

$\bar{M}_I$, $\bar{M}_{II}$, $\bar{M}_I$, $\bar{M}_{II}$	Partitioned matrices of $\tilde{M}$
N	Total number of stages
N_f	Feed stage
N_{IB}	Intermediate reboiler stage
N_{IC}	Intermediate condenser stage
P	Process transfer matrix of conventional column with respect to disturbance variables
P_{ij}	Elements of matrix P
P	Process transfer matrix of modified column with respect to disturbance variables
P_I, P_{II}	Partitioned matrices of P
q_b, Q_b	Intermediate boiler duty, K. Cals/min.
q_c, Q_c	Intermediate condenser duty, K. Cals/min.
Q_B	Main boiler duty, K. Cals/min.
Q_C	Main condenser duty, K. Cals/min.
R	Reflux ratio
R_m	Minimum reflux ratio
s	Laplace transformation parameter
T	Time in minutes
T_1, T_2, T_3	Time constants for elements of the transfer matrices
u	Control variables matrix for the conventional column
U	Control variables matrix for the modified column
U_I	Control variables matrix of case I of modified column
U_{II}	Control variables matrix of case II of modified column

v	Vapor flow from the intermediate reboiler, moles/min.
V	Main boil-up rate, moles/min.
$\bar{V}$	Internal vapor flow above the intermediate condenser stage, moles/min.
$\bar{\bar{V}}$	Internal vapor flow below intermediate condenser stage and above feed stage, moles/min.
V'	Internal vapor flow below feed stage and above intermediate boiler stage, moles/min.
V''	Internal vapor flow below intermediate boiler stage or main boil-up rate, moles/min.
V_r	Vapor flow from vapor space above rth stage, moles/min.
V_r'	Vapor flow from liquid on rth stage to vapor space above rth stage, moles/min.
w	Disturbance variables matrix
x	Controlled variables matrix of conventional column
x_r	Liquid composition at stage r
x_B	Bottoms product composition
x_D	Distillate composition
x^s	Set point matrix of the controlled variables
X	Controlled variables matrix of modified column
X_I	Controlled variables of case I of modified column
X_{II}	Controlled variables of case II of modified column

X^s	Set point matrix for the modified column
y_r	Vapor composition of stage r
y^*	Equilibrium vapor composition
z	Feed composition
ϵ_b	Error in intermediate boiler stage composition
ϵ_c	Error in intermediate condenser stage composition
α	Relative volatility
θ	Time delay parameter
τ_I	Integral time constant
ω_{co}	Cross over frequency