

DYNAMIC SIMULATION OF A MULTICOMPONENT DISTILLATION COLUMN

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INTRODUCTION

The study of the dynamic behavior of distillation columns has been one of the most interesting and challenging topics of process simulation in oil refinery and chemical industries. Since the pioneer work of Marshall and Pigford (1) in 1947 innumerable articles have been published on this subject. However, most of the work has been directed toward binary systems and relatively little effort has been devoted to the multicomponent systems due to the complexity of the process and the difficulty encountered in computations.

Among those studies in connection with binary distillations, Huckaba and his co-workers (2) and Gerster, et al. (3,4,5) are especially noted for their good experimental verification of mathematical models.

Peiser and Grover(6) were the first to present a detailed mathematical model for a multicomponent distillation column. The method used to solve the proposed model was not mentioned. Cadman(7) and Tranmontin(8) presented several linearized models with different degrees of complexity for control study. Holland and his co-workers (9,10,11) have done extensive work on digital simulation of multicomponent distillations. Iterative calculation procedures were employed to solve the tray temperatures and flow rates in their models. Snyder(12) developed direct calculation procedures to update all variables at each time increment. However, the equations and the solution method presented were limited to ideal solutions.

The objective of this study was to present a detailed, although not comprehensive, mathematical model for non-ideal multicomponent distillations and direct calculation procedures to solve the equations in the model. The model was generalized to handle multiple feeds, side draws, heaters and coolers and may be applied to other types of multistages separation processes such as absorption, strip-pings and batch distillations as well.

MATHEMATICAL MODEL

It is generally believed that a mathematical model for multicomponent distillations could be developed to any desired degree of complexity through experimental knowledge and theoretical insight. Due to the enormous complexity of multicomponent distillation processes, a very comprehensive mathematical model would mean a great deal of computing time which may not be of practical interest. In general, the ways of formulating mathematical models depend largely upon the purpose of application and the ability and efficiency of equipment available for solving the resulting models.

The following major assumptions were made in the derivation of the dynamic mathematical model of a multicomponent distillation column.

1. Negligible vapor holdup on each tray.
2. Perfect vapor mixing on each tray
3. Perfect liquid mixing on each tray.

Some other minor assumptions in the derivation can be easily eliminated by applying adequate equations which are accessible from related references.

The schematic diagram of a distillation column is shown in Figure 1.

Overall Material Balance

$$\frac{dM_j}{dt} = V_{j+1} + L_{j-1} - (V_j + W_j) - (L_j + U_j) + F_{j+1}^V + F_j^L \quad (1)$$

where the liquid holdup on tray j, M_j , is calculated as

$$M_j = A_j h_j \rho_j \quad (2)$$

Therefore,

$$\frac{dh_j}{dt} = \frac{1}{A_j \rho_j} [V_{j+1} + L_{j-1} - (V_j + W_j) - (L_j + U_j) + F_{j+1}^V + F_j^L] \quad 1 \leq j \leq N \quad (3)$$

Component Material Balance

$$\begin{aligned} \frac{dX_{i,j}}{dt} = \frac{1}{M_j} [& -A_j \rho_j X_{i,j} \frac{dh_j}{dt} + V_{j+1} y_{i,j+1} + L_{j-1} X_{i,j-1} \\ & - (V_j + W_j) y_{i,j} - (L_j + U_j) X_{i,j} + F_{j+1}^V y_{i,j+1}^F \\ & + F_j^L X_{i,j}^F] \quad 1 \leq i \leq n, \quad 1 \leq j \leq N \quad (4) \end{aligned}$$

Enthalpy Balance

The enthalpy balance equations which are used to solve for vapor flow rate equations are given in the Appendix.

Vapor Liquid Equilibrium

$$y_{i,j} = E_{i,j} k_{i,j} X_{i,j} \quad (5)$$

Where $k_{i,j}$ is the vapor-liquid equilibrium ratio for component i on tray j and is a function of temperature, pressure and liquid composition. $E_{i,j}$ is the tray efficiency.

Bubble Point Temperature

$$\frac{dT_j}{dt} = C_j^1 + C_j^2 (V_j + W_j) + C_j^3 V_{j+1} \quad (6)$$

The derivations of Equation (6) are given in the Appendix. If the reflux is subcooled, its temperature is determined separately according to a prescribed fashion.

Liquid Flow Rates

Using the Francis weir formula the liquid flow rate from tray j down to the next tray is

$$L_j = \alpha \left(\frac{h_j - l_j}{\beta} \right)^{1.5} \quad 2 \leq j \leq N-1 \quad (7)$$

where α and β are constants which depend on the length of the perimeter of downcomer and the liquid molal density, and l_j is the weir height on tray j .

Vapor Flow Rates

$$V_j = (d_j' + d_j^3 V_{j+1}) / d_j^2 \quad 1 \leq j \leq N \quad (8)$$

The derivations of Equation (8) are given in the Appendix.

Distillate or Reflux Flow Rate

The distillate or reflux flow rate is subjected to manipulation by a feedback and/or feedforward controller. When manipulating reflux flow rate, the distillate flow rate is controlled by a liquid level controller. Using a proportional-integral controller for the liquid level control of the accumulator, the distillate flow rate can be expressed as,

$$\frac{dU_1}{dt} = K_1 \left(\frac{dh_1}{dt} + \frac{h_1 - h_1^0}{I_1} \right) \quad (9)$$

where K_1 is a combined constant which includes the controller and process gains, and I_1 is the reset time; h_1 and h_1^0 are the current and steady state heights of liquid levels respectively in the accumulator.

Bottom Product Flow Rate

The bottoms flow rate or the reboiler heat is subjected to manipulation of a feedback and/or feedforward controller. In most cases, reboiler heat is used to control the bottom product composition and the bottom flow rate is controlled by a liquid level controller on the reboiler. Again, for a PI mode controller the bottoms flow rate can be expressed as

$$\frac{dL_N}{dt} = K_N \left(\frac{dh_N}{dt} + \frac{h_N - h_N^0}{I_N} \right) \quad (10)$$

For given feed rate conditions, reflux rate and reboiler heat, there are $N(n+2)+2$ differential equations and $2N-2$ algebraic equations to solve for $N(n+4)$ unknowns, i.e., $X_{i,j}$, h_j , T_j , V_j , L_j , and U_1 at each time increment.

CALCULATIONAL PROCEDURES

The calculational procedures for solving the model are as follows:

1. Read initial conditions. These may be steady state conditions or any arbitrary conditions.
2. Calculate bubble point temperatures corresponding to the given liquid compositions by conventional iterative methods. This step is not necessary if the equilibrium temperatures are given as initial conditions.
3. Use Equation (7) to calculate liquid flow rates if initial liquid heights are given. Otherwise, calculate liquid heights if initial flow rates are given.
4. Calculate vapor flow rates from Equation (8) starting from the reboiler and progressing upward to the top tray of the column.
5. Integrate Equations (3), (4), (6), (9) and (10) to give h_j , $X_{i,j}$, T_j , U_1 and L_N for the next time increment.
6. Calculate liquid and vapor flow rates from Equations (7) and (8).
7. Repeat procedures (5) and (6) until the termination condition is satisfied.

INTEGRATION METHOD AND STEP SIZE

Different integration methods such as the Euler method (13,14,15), the implicit method (9,16), the Runge-Kutta method (12,17), and the predictor-corrector method (2,18) have been used to solve the dynamic behavior of distillation columns. Franks⁽¹⁹⁾ reported that contrary to a small system where a large time step size and higher order of integration method results in a more efficient solution, the critical step sizes for stability are of the same order of magnitude for all integration methods, when a large system (50-500 differential equations) is involved. He indicated that the fourth order Runge-Kutta critical step size was only about fifty percent greater than for the simple Euler method. Using the Euler method near the critical step size provides a stable and reasonably accurate solution.

The Euler method was adopted for integration after comparing the critical step size and the results from employing a Runge-Kutta method and a simple Euler method. Depending upon the magnitude of the disturbance, the critical step size is about 3.6 seconds for the fourth order Runge-Kutta method and is approximately 2.5 seconds for the Euler method (20). A time step size of 1.8 seconds was used for this study.

The computing times required for each time increment are given in Table I. For one hour real time simulation it requires about 1.2 minutes of CPU time on an IBM 370/168 digital computer for a twenty-tray column separating a five component system. It was found that the computing time was roughly proportional to the number of trays and number of components.

TABLE I. Computing time for each step
CPU Time

No. of Comp.	No. of Trays	Method	Integration for Each Step, Sec.	Computer	Reference
3	7	Implicit	11.4	IBM709	(9)
3	7	Runge-Kutta	3.9	IBM7090	(12)
5	10	Euler	0.06	IBM360/65	(20)
				(H Compiler)	
5	20	Euler	0.036	IBM370/168	This Work
				(G Compiler)	

PROCESS REACTION CURVES

A twenty-tray column, five feet in diameter, separating a five component system, namely propane, iso-butane, n-butane, iso-pentane, and n-pentane, was simulated on a digital computer to investigate the process dynamics of multicomponent distillations. The detailed column configuration is given in Table 2. The vapor-liquid equilibrium ratios and enthalpy data are from Reference 21. The column steady-state conditions are given in Tables 3 and 4.

The responses of top and bottom product compositions to step changes in feed rate are shown in Figures 2 and 3. The normalized response curves for feed rate and/or feed composition changes are shown in Figures 4 and 5. As can be seen, the multicomponent distillation process is highly non-linear. The shapes of the process reaction curves not only vary with the magnitude of the disturbance but also the direction (positive or negative) of the disturbance as well. Feed composition changes make the overall system performance even more complicated. In viewing these, it would be difficult to develop column transfer functions which could relate the input and output variables satisfactorily. This also indicates that the validity of the models obtained from linearization of the system's differential equations around a steady state condition is doubtful for larger disturbances.

TABLE 2 Column Configuration

Number of trays = 20
 Feed tray number = 11
 Column diameter = 5 feet
 Length of overflow weir = 3.75 feet
 Height of overflow weir = 0.25 feet
 Plate floor area = 15.2 ft.²
 Cross-sectional area of downcomer = 2.2 ft.²
 Liquid holdup in reflux drum = 62.4 moles
 Liquid holdup in reboiler = 124.8 moles
 $K_1 = 200$ moles/ft.
 $I_1 = 0.1$ hour
 $K_N = 450$ moles/ft.
 $I_N = 0.1$ hour

TABLE 3 Steady-State Conditions

Column pressure = 120 psia
 Feed flow rate = 600 moles/hour
 Feed temperature = 194.64°F (Bubble Point)
 Distillate flow rate = 229.22 moles/hour
 Reflux flow rate = 930 moles/hour
 Reflux temperature = 151.83°F (Bubble Point)
 Reboiler heat = 9606437 BTU/hour

Component	Feed Composition	
	Steady-State	Step Change*
Propane	0.01	0.01
isc-butane	0.18	0.18
n-butane	0.20	0.16
iso-pentane	0.28	0.32
n-pentane	0.33	0.33

Component	Distillate	Bottoms
Propane	0.02617	0.
iso-butane	0.46845	0.00167
n-butane	0.49850	0.01543
iso-pentane	0.00592	0.44947
n-pentane	0.00096	0.53343

TABLE 4 Steady-State Conditions

Tray No.	Temp., °F	Vapor Flow Rate, Mol/Hr.	Liquid Flow Rate, Mol/Hr.
1			930.0
2	151.8	1159.2	924.7
3	154.6	1153.9	916.1
4	157.5	1145.3	903.5
5	161.2	1132.7	886.2
6	166.2	1115.4	864.9
7	172.9	1094.1	842.7
8	180.6	1071.9	823.7
9	188.5	1053.0	810.0
10	195.5	1039.5	802.0
11	200.9	1031.2	1401.4
12	206.7	1030.6	1401.7
13	212.4	1030.9	1403.6
14	217.7	1032.9	1406.9
15	222.3	1036.2	1411.0
16	226.2	1040.2	1414.9
17	229.3	1044.1	1418.2
18	231.7	1047.4	1420.5
19	233.6	1049.7	1421.9
20	235.2	1051.1	370.8

The effects of the tray hydraulics and the energy balance are shown in Figures 6-9. Again, the normalized response curves were plotted. Three different cases were

*For a step change in feed composition. The feed temperature is 198.05°F (Bubble Point).

studied. First, the tray hydraulics was not included (Curve B). The liquid holdup on each tray remains unchanged when the column is subjected to disturbance. The liquid flow rates will respond to feed rate change instantaneously. In this case, constant liquid levels in both the accumulator and the reboiler were also assumed. Second, the energy effect was not included (Curve C). The vapor flow rates stay constant regardless of the disturbance. Third, both the effects of the tray hydraulics and the energy balance were not considered (Curve D). The deviations of compositions of the light key and the heavy key components from their original steady state conditions are given in Table 5.

From Figures 6-9 and Table 5, it can be seen that the exclusion of the effects of the tray hydraulics and/or the energy balance not only change the steady-state compositions toward new conditions, but also vary the shapes of responses. For constant holdup, it responds the fastest and tends to be of lower order system due to instantaneous change of liquid flows. For constant vapor flow rate, it experiences the slowest response. For constant liquid holdup and vapor flow rate, the response is somewhat in between the above two, depending on which one is predominant.

TABLE 5 Deviations of Compositions From Original Steady-State Conditions

Step Change	Heavy key in Distillate (i-C ₅), mole fraction	Light key in Bottoms (n-C ₄), mole fraction
+20% Feed Rate(A)	-0.0044	0.0670
+20% Feed Rate(B)	-0.0051	0.1251
+20% Feed Rate(C)	-0.0045	0.0763
+20% Feed Rate(D)	-0.0041	0.0765
-10% Feed Rate(A)	0.0264	-0.0099
-10% Feed Rate(B)	0.0440	-0.0109
-10% Feed Rate(C)	0.0663	-0.0111
-10% Feed Rate(D)	0.0665	-0.0112

- (A) Variable liquid holdup and vapor flow rate
- (B) Constant liquid holdup
- (C) Constant vapor flow rate
- (D) Constant liquid holdup and vapor flow rate

The response curves shown in Figures 4-9 may only apply to the system studied. Different conditions such as feed stream conditions (temperature and vapor-liquid ratio) highly non-ideal solution, and extremely wide or narrow boiling point system may result in different situations. Nonetheless, it reveals the significance of the consideration of the tray hydraulics and energy effect. Considerable care must be taken to ensure the adequacy of the mathematical model formulated before applying it to the system of interest.

CONCLUSIONS

A detailed dynamic mathematical model which includes the tray hydraulics, and non-linear equilibrium and energy effects, was developed for process dynamics and control studies of multicomponent distillation columns. The model developed is applicable to non-ideal systems. Instead of using an iteration technique, direct calculation procedures were developed to calculate the transient equilibrium tray temperatures and the vapor flow rates throughout the column. It requires about 1.2 minutes for one hour real time simulation for a twenty-tray column separating a five component system on an IBM 370/168 digital computer.

The model was demonstrated by simulating a de-butanizer. Considerable non-ideality of the process was observed. The effect of the tray hydraulics and energy balance was also shown to be significant in the dynamic simulation of multicomponent distillation columns.

NOMENCLATURE

A_j	Tray j floor area, ft
$a_{i,j}^1, a_{i,j}^2, a_{i,j}^3$	Variables defined by Equations (A-2), (A-3), (A-4) respectively
b_j^1, b_j^2, b_j^3	Variables defined by Equations (A-16), (A-17), (A-18) respectively
$c_{j,i}^1, c_{j,i}^2, c_{j,i}^3$	Variables defined by Equations (A-10), (A-11), (A-12), (A-13) respectively
d_j^1, d_j^2, d_j^3	Variables defined by Equations (A-23), (A-24), (A-25) respectively
E	Tray efficiency
F_j	Feed stream at tray j, moles/hour
G_j	Molal enthalpy of the vapor stream V_j , BTU/mole
H_j	Molal enthalpy of the liquid stream L_j , BTU/mole
\bar{H}_j	Partial molal enthalpy of component i in the liquid stream L_j , BTU/mole
h_j	Average height of the liquid holdup on tray j, ft
I	Reset time, hour
K_1	Constant defined by Equation (9)
K_N	Constant defined by Equation (10)
$k_{i,j}$	Vapor-liquid equilibrium ratio of component i at tray j
L_j	Liquid stream flowing from the jth tray down to the (j+1)th tray, moles/hour (L_1 is the reflux flow rate)
l_j	Height of overflow weir, ft.
M_j	Total liquid holdup on tray j, moles
N	Number of trays including condenser and reboiler
n	Number of components
P_j	Pressure at tray j, psia
Q_j	Heat duty of the tray j, BTU/hour (Q_1 and Q_N are the heat duties of the condenser and the reboiler respectively)
T_j	Temperature at tray j, deg. F
t	Time, hour
U_j	Liquid side draw from tray j, moles/hour (U_1 is the overhead liquid product)
V_j	Vapor stream leaving the jth tray to the (j-1)th tray above, moles/hour (V_1 is the overhead vapor product)
W_j	Vapor side draw from tray j, moles/hour
$x_{i,j}$	Mole fraction of component i in the liquid stream leaving tray j
$y_{i,j}$	Mole fraction of component i in the vapor stream V_j

GREEK LETTERS

α	Constant defined by Equation (7)
β	Constant defined by Equation (7)
ρ	Liquid molal density, moles/cu.ft.

SUBSCRIPTS

1	First tray or condenser
i	Component number
j	Tray number
m	Component number
N	Last tray or reboiler

SUPERSCRIPTS

o	Steady-state value
F	Feed stream
L	Liquid in the feed stream
V	Vapor in the feed stream
*	Used to define $V_j^* = V_j + W_j$

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APPENDIX

Component material balance Substituting Equation(3) into Equation(4) and after rearrangement gives

$$\frac{d\chi_{i,j}}{dt} = a'_{i,j} + a''_{i,j} V_j^* + a'''_{i,j} V_{j+1} \quad (A-1)$$

where
$$a'_{i,j} = \frac{1}{M_j} [L_{j-1}(\chi_{i,j-1} - \chi_{i,j}) + F_{j+1}^V(y_{i,j+1}^F - \chi_{i,j}) + F_j^L(\chi_{i,j}^F - \chi_{i,j})] \quad (A-2)$$

$$a''_{i,j} = \frac{1}{M_j} [\chi_{i,j} - y_{i,j}] \quad (A-3)$$

$$a'''_{i,j} = \frac{1}{M_j} [y_{i,j-1} - \chi_{i,j}] \quad (A-4)$$

and
$$V_j^* = V_j + W_j \quad (A-5)$$

Bubble point temperature The bubble point temperature requires the summation of vapor compositions at each tray to be unity, i.e.,

$$\sum_{i=1}^n y_{i,j} = 1 \quad (A-6)$$

For a tray efficiency of 100 % ($E_{i,j}=1$), the bubble point temperature equation becomes

$$\sum_{i=1}^n k_{i,j} \chi_{i,j} = 1 \quad (A-7)$$

The vapor-liquid equilibrium ratio, $k_{i,j}$, is a function of temperature, pressure, and liquid composition. Differentiating Equation(A-7) with respect to time and applying the chain rule of differentiation yields

$$\sum_{i=1}^n k_{i,j} \frac{d\chi_{i,j}}{dt} + \sum_{i=1}^n \chi_{i,j} \left[\frac{\partial k_{i,j}}{\partial T_j} \frac{dT_j}{dt} + \frac{\partial k_{i,j}}{\partial P_j} \frac{dP_j}{dt} + \sum_{m=1}^n \frac{\partial k_{i,j}}{\partial \chi_{m,j}} \frac{d\chi_{m,j}}{dt} \right] = 0 \quad (A-8)$$

When the column is subjected to disturbances, the change of pressure at each tray is comparatively small. Since the effect of pressure on the vapor-liquid equilibrium ratio is not as pronounced as that of temperature, the pressure variation term, dP_j/dt , will be neglected for the purposes of dynamic simulation.

Substituting Equation(A-1) into Equation(A-8) and solving for dT_j/dt yields

$$\frac{dT_j}{dt} = C_j^1 + C_j^2 V_j^* + C_j^3 V_{j+1} \quad (A-9)$$

where
$$C_j^0 = -\sum_{i=1}^n \chi_{i,j} \left(\frac{\partial k_{i,j}}{\partial T_j} \right) \quad (A-10)$$

$$C_j^1 = \frac{1}{C_j^0} \left[\sum_{i=1}^n k_{i,j} a'_{i,j} + \sum_{i=1}^n \chi_{i,j} \sum_{m=1}^n \left(\frac{\partial k_{i,j}}{\partial \chi_{m,j}} \right) a'_{m,j} \right] \quad (A-11)$$

$$C_j^2 = \frac{1}{C_j^0} \left[\sum_{i=1}^n k_{i,j} a''_{i,j} + \sum_{i=1}^n \chi_{i,j} \sum_{m=1}^n \left(\frac{\partial k_{i,j}}{\partial \chi_{m,j}} \right) a''_{m,j} \right] \quad (A-12)$$

$$C_j^3 = \frac{1}{C_j^0} \left[\sum_{i=1}^n k_{i,j} a'''_{i,j} + \sum_{i=1}^n \chi_{i,j} \sum_{m=1}^n \left(\frac{\partial k_{i,j}}{\partial \chi_{m,j}} \right) a'''_{m,j} \right] \quad (A-13)$$

Enthalpy balance The enthalpy balance equation for tray j can be written as

$$\frac{dM_j H_j}{dt} = V_{j+1} G_{j+1} + L_{j-1} H_{j-1} - (V_j + W_j) G_j - (L_j + U_j) H_j + F_{j+1}^V G_{j+1}^F + F_j^L H_j^F + Q_j \quad (A-14)$$

where Q_j is positive for heating and negative for cooling.

Similar to the derivation of Equation(A-1), the energy balance equation can be expressed as

$$\frac{dH_j}{dt} = b_j^1 + b_j^2 V_j^* + b_j^3 V_{j+1} \quad (A-15)$$

where
$$b_j^1 = \frac{1}{M_j} [L_{j-1}(H_{j-1} - H_j) + F_{j+1}^V(G_{j+1}^F - H_j) + F_j^L(H_j^F - H_j) + Q_j] \quad (A-16)$$

$$b_j^2 = \frac{1}{M_j} [H_j - G_j] \quad (A-17)$$

$$b_j^3 = \frac{1}{M_j} [G_{j+1} - H_j] \quad (A-18)$$

The liquid molal enthalpy, H_j , is calculated from the partial molal enthalpies by

$$H_j = \sum_{i=1}^n \bar{H}_{i,j} \chi_{i,j} \quad (A-19)$$

Differentiating Equation(A-19) with respect to time yields

$$\frac{dH_j}{dt} = \sum_{i=1}^n \bar{H}_{i,j} \frac{d\chi_{i,j}}{dt} + \sum_{i=1}^n \chi_{i,j} \left[\frac{\partial \bar{H}_{i,j}}{\partial T_j} \frac{dT_j}{dt} + \frac{\partial \bar{H}_{i,j}}{\partial P_j} \frac{dP_j}{dt} + \sum_{m=1}^n \frac{\partial \bar{H}_{i,j}}{\partial \chi_{m,j}} \frac{d\chi_{m,j}}{dt} \right] \quad (A-20)$$

Again, neglecting dP_j/dt and substituting Equation (A-1) into Equation(A-20) gives

$$\begin{aligned} \frac{dH_j}{dt} = & \sum_{i=1}^n \bar{H}_{i,j} (a'_{i,j} + a''_{i,j} V_j^* + a'''_{i,j} V_{j+1}) + \\ & \sum_{i=1}^n \chi_{i,j} \left(\frac{\partial \bar{H}_{i,j}}{\partial T_j} \right) (C_j^1 + C_j^2 V_j^* + C_j^3 V_{j+1}) + \\ & \sum_{i=1}^n \chi_{i,j} \sum_{m=1}^n \left(\frac{\partial \bar{H}_{i,j}}{\partial \chi_{m,j}} \right) (a'_{m,j} + a''_{m,j} V_j^* + a'''_{m,j} V_{j+1}) \end{aligned} \quad (A-21)$$

Equating Equation(A-21) to Equation(A-15), the vapor flow rate, V_j , becomes

$$V_j^* = V_j + W_j = (d_j^1 + d_j^3 V_{j+1}) / d_j^2 \quad (A-22)$$

where
$$d_j^1 = \sum_{i=1}^n \bar{H}_{i,j} a'_{i,j} + \sum_{i=1}^n \chi_{i,j} \left(\frac{\partial \bar{H}_{i,j}}{\partial T_j} \right) C_j^1 + \sum_{i=1}^n \chi_{i,j} \sum_{m=1}^n \left(\frac{\partial \bar{H}_{i,j}}{\partial \chi_{m,j}} \right) a'_{m,j} - b_j^1 \quad (A-23)$$

$$d_j^2 = - \left(\sum_{i=1}^n \bar{H}_{ij} a_{ij}^2 + \sum_{i=1}^n \chi_{ij} \left(\frac{\partial \bar{H}_{ij}}{\partial T_j} \right) C_j \right) + \sum_{i=1}^n \chi_{ij} \sum_{m=1}^n \left(\frac{\partial \bar{H}_{ij}}{\partial \chi_{mj}} \right) a_{mj}^2 b_j^2 \quad (A-24)$$

$$d_j^3 = \sum_{i=1}^n \bar{H}_{ij} a_{ij}^3 + \sum_{i=1}^n \chi_{ij} \left(\frac{\partial \bar{H}_{ij}}{\partial T_j} \right) C_j^3 + \sum_{i=1}^n \chi_{ij} \sum_{m=1}^n \left(\frac{\partial \bar{H}_{ij}}{\partial \chi_{mj}} \right) a_{mj}^3 b_j^3 \quad (A-25)$$

For the last tray or reboiler, Equation(A-22) becomes

$$V_N + W_N = d_N' / d_N^2 \quad (A-26)$$

Equation(A-26) can be solved directly. Therefore, starting with Equation(A-26) the vapor flow rates throughout the column can be calculated using Equation(A-22).

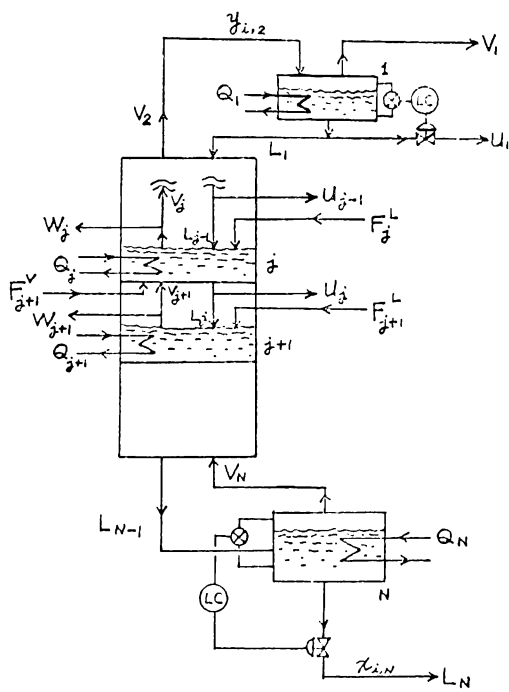


FIGURE 1

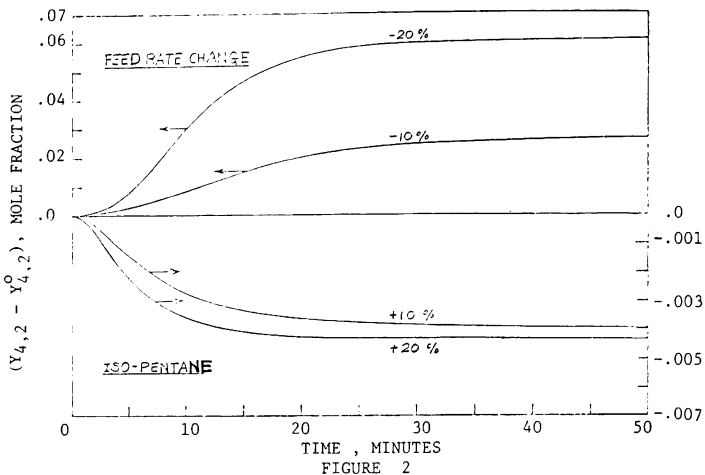


FIGURE 2

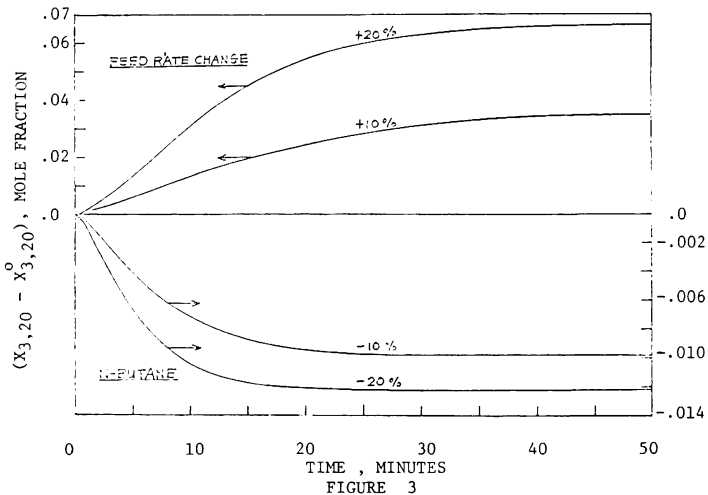


FIGURE 3

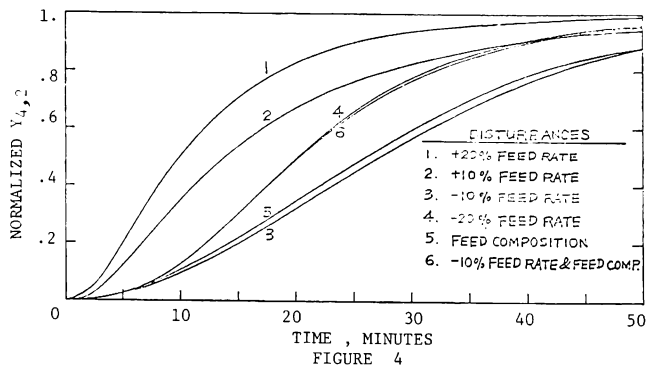


FIGURE 4

