

Dynamics of Fractional Distillation

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One of the numerous equations needed to define the dynamics of a distillation column has been derived. This equation relates the feed composition to the product composition. The derivation is accomplished by the reduction of the signal flow diagram. The poles and zeros of the equation are almost entirely determined by the ratio of the tray holdup to the liquid flow rates and the number of trays.

In order to study the control of any process it is desirable to have the equation representing the dynamic action of the process in factored form, where both the numerator and denominator may be made up of real and complex terms, as shown in Equation (1):

$$G(s) = \frac{K(s + z_1)(s + z_2) \dots (s + z_n)}{(s + p_1)(s + p_2) \dots (s + p_n)} \quad (1)$$

Equations of this form allow one to study the control of the process by any of several standard methods.

The complete analysis of a distillation column requires eight to ten equations of the form stated above which would represent the effect of the numerous inputs upon the product composition. Some of these input variables are the feed composition, temperature, flow rate and state (vapor or liquid), the reflux-flow rate and temperature, and the steam-flow rate and column pressure. The input variables having only a small effect need not be considered in the control studies. In this paper the equations relating the effect of the feed composition upon the product composition have been derived.

The start up of a fractionating column has been discussed by a number of authors (3). The conditions at start up are somewhat different than when the column is being controlled. For control studies it is necessary to know the effect of small disturbances when the process is operating at steady state. Wilkinson and Armstrong (3) and Voetter (2) have considered the problem of transients for simplified

cases. Both of these papers also give other references to fractionating column dynamics.

Williams et al. (4) studied the control of a distillation column with an analogue computer. Their work was limited to a maximum of five trays because of the large number of integrators needed. In order to study a column with 15 or 20 trays a very large and expensive computer would be needed. Therefore it seems desirable to investigate other methods of analysis. The method described below is not limited to any specific number of trays, and no computer is needed. The calculations become somewhat more laborious as the number of trays increases.

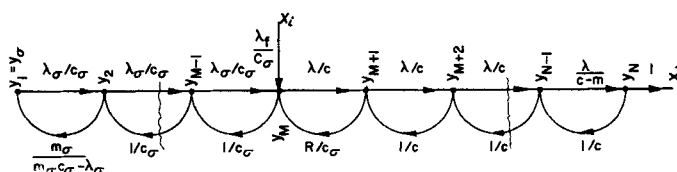
It is not difficult to set up the equations for the simplified column. The real problem is to reduce these equations to the form of Equation (1). There are a number of methods of performing this task, with the calculus of finite differences being perhaps most often used. In the following the signal flow diagram will be used to derive the equation for two reasons. It is believed the method will be useful to chemical engineers in other problems, with distillation being an ex-

cellent example, and the signal flow diagram show more clearly the effect of the column parameters upon the final equation than abstract mathematical methods. Teager (6) and Campbell (5) suggest the use of signal flow diagrams for distillation and present a general diagram for a column. Campbell does not give the complete reduction of the diagram or a numerical example.

DERIVATION OF EQUATIONS

The operating conditions assumed are:

1. Only small disturbances are considered so that linearized equations can be used.
2. The vapor holdup is small and therefore neglected.
3. The plate efficiency is 100%.
4. Fluid flow and heat dynamics are neglected.
5. The vapor liquid equilibrium is linear, with a separate equilibrium line for the stripping and enriching sections.
6. There are constant molal flows of the vapor and liquid.
7. When $t=0$, the column is at steady state.
8. The feed enters as liquid at the boiling point.
9. There is no holdup in the condenser.
10. The reboiler has the same holdup as the trays.



A mass balance around the n th tray in the enriching section is

$$L x_{n+1} + V y_{n-1} - L x_n - V y_n = C \frac{dx_n}{dt} \quad (2)$$

Then since $y_n = m x_n$, Equation (2) becomes

$$\frac{L}{m} y_{n+1} + V y_{n-1} - \frac{L}{m} y_n - V y_n = C \frac{dy_n}{dt} \quad (3)$$

Divide by L/m ; then

$$y_{n+1} = \frac{Vm}{L} y_{n-1} - y_n - \frac{Vm}{L} y_n = \frac{Vm}{L} y_n = \frac{C}{L} \frac{dy_n}{dt} \quad (4)$$

When one takes the Laplace transform and makes substitutions for the coefficients, Equation (4) becomes

$$\bar{y}_{n+1} + \lambda \bar{y}_{n-1} - c \bar{y}_n = 0 \quad (5)$$

At the top of the column a mass balance after transformation and substitution for the coefficients becomes

$$\bar{y}_n = \frac{\lambda}{c-m} \bar{y}_{n-1} \quad (6)$$

In the stripping section

$$\bar{y}_{m+1} + \lambda \bar{y}_{m-1} - c \bar{y}_m = 0 \quad (7)$$

At the bottom of the column

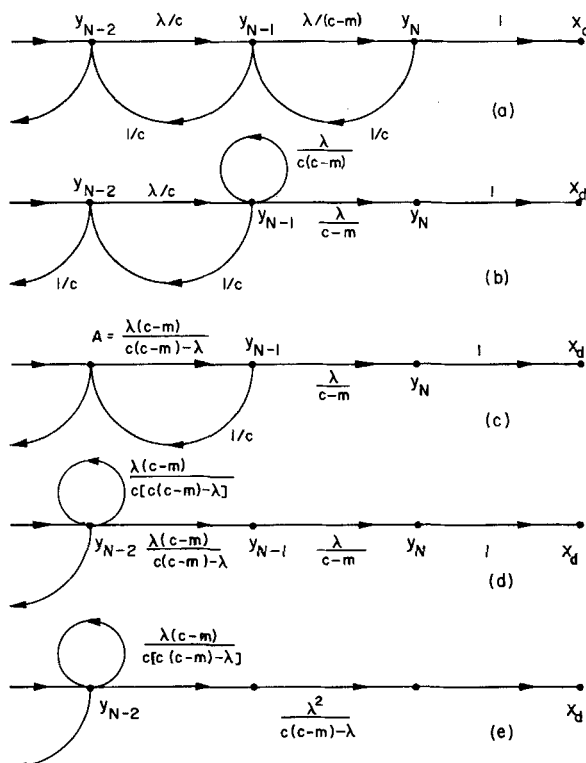


Fig. 2. Reduction of the signal flow diagram for the enriching section.

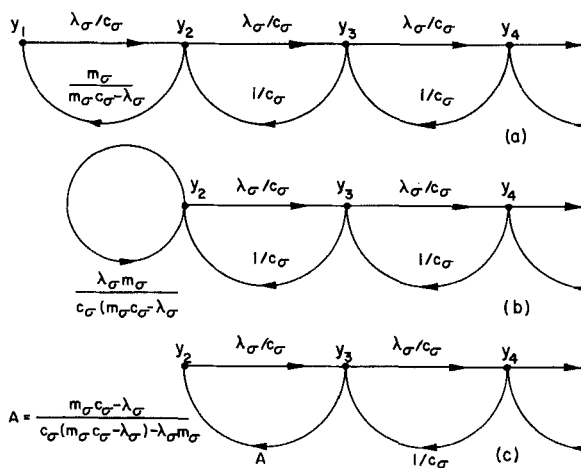


Fig. 3. Reduction of the signal flow diagram for the stripping section.

$$\bar{y}_1 = \frac{m_\sigma}{m_\sigma c_\sigma - y_\sigma} \bar{y}_2 \quad (8)$$

At the feed tray which is the M th tray including the reboiler as a tray

$$\lambda_f \bar{x}_i + R \bar{y}_{M+1} + \lambda_\sigma \bar{y}_{M-1} - c_\sigma \bar{y}_M = 0 \quad (9)$$

THE SIGNAL FLOW DIAGRAM

The signal flow diagram can now be drawn as shown in Figure 1. The composition of the vapor from each tray is indicated by y and the distillate composition $y_N = x_d$. The equation representing the vapor composition on each tray is the sum of all the signals en-

tering the point or node. The terms on each line are the transfer functions that give the input-output relationship between the quantities on the ends of the line. For example

$$\bar{y}_{m+1} = (\lambda/c) \bar{y}_m + \frac{1}{c} \bar{y}_{m+2}$$

The reduction of this diagram is accomplished by a few simple rules. Truxal (1) and Campbell (5) give good descriptions of the signal flow diagrams.

Beginning at the top of the column one can proceed one tray at a time. It is obvious that Figures 2a and 2b are equivalent, since in Figure 2a

$$\bar{y}_{N-1} = (1/c) \bar{y}_N + (\lambda/c) \bar{y}_{N-2}$$

and

$$\bar{y}_N = \frac{\lambda}{c-m} \bar{y}_{N-1}$$

therefore

$$\bar{y}_{N-1} = \frac{\lambda}{c(c-m)} \bar{y}_{N-1} + (\lambda/c) \bar{y}_{N-2}$$

The loop at y_{N-1} can be combined with the signal entering y_{N-1} as follows:

$$\frac{\bar{y}_{N-1}}{\bar{y}_{N-2}} = A = \frac{\lambda/c}{1 - \frac{\lambda}{c(c-m)}} = \frac{\lambda(c-m)}{c(c-m) - \lambda} \quad (10)$$

as shown in Figure 2c.

The next step is to eliminate the return signal y_{N-1} to y_{N-2} as shown in Figure 2d. The process is repeated until the feed tray is reached. The functions between each tray are the transfer functions relating the composition of one tray to that of the tray above. These can be combined by multiplication to give the transfer function between any two trays. For example in Figure 2e, from tray y_{N-2} to x_d , the transfer function is

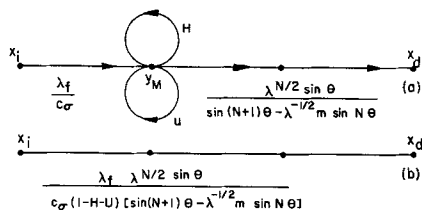


Fig. 4. Reduced signal flow diagram.

$$\bar{x}_d = \frac{\lambda(c-m)}{c(c-m) - \lambda} \frac{\lambda}{c-m} \bar{y}_{N-2} = \frac{\lambda^2}{c(c-m) - \lambda} \bar{y}_{N-2} \quad (11)$$

If one studies the equations developed in the reduction, it can be seen that a definite pattern is followed, so that one can write down each term without any calculation.

Now let

$$c = 2\sqrt{\lambda} \cos \theta$$

$$\theta = \tan^{-1} \frac{1}{c} \sqrt{4\lambda - c^2} \quad (11a)$$

Then it can be shown that for the N trays in the enriching section the transfer function is

$$\bar{y}_N = \frac{\lambda^{N/2} \sin \theta}{\sin(N+1)\theta - \left(\frac{m}{\lambda^{1/2}}\right) \sin N\theta} \bar{y}_M \quad (12)$$

where N is the number of trays above the feed tray and y_M the composition of the vapor from the feed tray.

After each step in the reduction there is a loop formed at the tray from which the return signal has been removed. When one makes the substitution given in Equation (11a), the general equation for the loop function H for the N trays in the enriching section is

$$H = \frac{\lambda^{1/2} R [\sin N\theta - (m/\lambda^{1/2}) \sin(N-1)\theta]}{c_\sigma [\sin(N+1)\theta - (m/\lambda^{1/2}) \sin N\theta]} \quad (13)$$

The reduction of the diagram for the stripping section proceeds in the same manner. The steps are shown in Figure 3. The original diagram is shown in Figure 3a. The elimination of y_1 is shown in Figure 3b. Then the loop is eliminated by

$$A = \frac{1/c_\sigma}{1 - \frac{m_\sigma \lambda_\sigma}{c_\sigma(m_\sigma c_\sigma - \lambda_\sigma)}} = \frac{m_\sigma c_\sigma - \lambda_\sigma}{c_\sigma(m_\sigma c_\sigma - \lambda_\sigma) - \lambda_\sigma m_\sigma} \quad (14)$$

When the process is completed, it will

be found that the diagram appears as in Figure 4a. The second loop U is due to the stripping section. When one makes the substitution of Equation (11a), the general equation for the loop U is

$U =$

$$\frac{\lambda_\sigma^{1/2} [m_\sigma \sin M\phi - \lambda_\sigma^{1/2} \sin(M-1)\phi]}{c_\sigma [m_\sigma \sin(M+1)\phi - \lambda_\sigma^{1/2} \sin M\phi]} \quad (15)$$

The two loops and the equation for the stripping section can now be combined to give the over-all equation:

$$\bar{x}_d = \frac{\lambda_f c_\sigma}{1 - H - U} \frac{\lambda^{N/2} \sin \theta}{\sin(N+1)\theta - (m/\lambda^{1/2}) \sin N\theta} \bar{x}_i = \frac{\lambda^{N/2} \lambda_f c_\sigma [m_\sigma \sin(M+1)\phi - \lambda_\sigma^{1/2} \sin M\phi] \sin \theta}{H_j U_j - H_i U_j - H_j U_i} \bar{x}_i \quad (16)$$

where H_i and U_i are the numerators and H_j and U_j the denominators of the loop functions H and U .

If one were interested in the bottoms composition, the same procedure for the reduction process could be used to obtain the relationship between the feed composition and the bottoms composition.

The zeros and poles are not obvious in an equation of the form of Equation (16). The method of converting to the form of Equation (1) will be shown in the illustration to follow.

The steady state after a step input or the zero frequency amplitude ratio can be calculated from Equation (16). From the final value theorem the steady state is obtained by letting $s = 0$. From Equation (11a)

$$\theta = \tan^{-1} \frac{1}{c} \sqrt{4\lambda - c^2} = \tan^{-1} \frac{\sqrt{4\lambda - (\alpha s + 1 + \lambda)^2}}{\alpha s + 1 + \lambda}$$

When $s = 0$

$$\theta_{s=0} = \tan^{-1} \frac{\sqrt{4\lambda - (1 + \lambda)^2}}{1 + \lambda}$$

Upon substitution of $\theta_{s=0}$ and $\phi_{s=0}$ into Equation (16) the steady state value is obtained. When $\lambda \neq 1$, the term under the radical is negative. When this occurs all of the trigonometric terms above and in Equation (16) are changed to hyperbolic functions.

ILLUSTRATION

The responses of the column to any type of input or feed change can be calculated from Equation (16). There are a number of methods of performing this calculation; however it seems best to first find the specific poles and zeros of the function. This can be shown by a numerical ex-

ample. Let the various parameters have the following values:

TABLE 1

$m = 0.855$	$m_\sigma = 1.38$
$\lambda = 2.10$	$\lambda_\sigma = 1.0$
$\alpha = 0.396$	$\alpha_\sigma = 0.117$
$R = 0.477$	$\lambda_f = 0.97$
$N = 5$	$M = 4$

The zeros of Equation (16) are obtained by solving the numerator for values of ϕ which make the numerator equal to 0. That is upon substitution of numbers into the term in the brackets

$$\sin 5\phi - 0.724 \sin 4\phi = 0 \quad (17)$$

Values of ϕ satisfying Equation (17) are

most easily found by plotting the curve $\frac{\sin 5\phi}{\sin 4\phi}$ from 0 to $\pi/2$ and picking off the

values at which the curve crosses the ordinate 0.724. The curve could be plotted from 0 to π , but this is not necessary since the curves from $\pi/2$ to π are the same as the curves from 0 to $\pi/2$ reflected in a vertical line at $\pi/2$ followed by a reflection in the x axis. The values of the zeros are found from Equation (11a):

$$2\lambda^{1/2} \cos \phi = c_\sigma = 1 + \lambda_\sigma + \alpha_\sigma s$$

or

$$s = \frac{2\lambda_\sigma^{1/2} \cos \phi - 1 - \lambda_\sigma}{\alpha_\sigma} = \frac{2 \cos \phi - 2}{0.186} \quad (18)$$

The specific values are given in Table 2.

In the conversion from the trigonometric form to the form exhibiting the roots of the polynomials it is necessary to factor out the terms λ and α . In addition each of the terms in the brackets of Equation (16) has associated with it a $\sin \theta$ or $\sin \phi$ term. All of the sine terms cancel except $\sin \theta$. For example

$$\frac{\sin 5\phi - 0.724 \sin 4\phi}{\sin \phi} = \alpha_\sigma^4 \lambda_\sigma^2 (s + 1.16) (s + 5.87) (s + 15.03) (s + 18.2)$$

In other words $\alpha_\sigma^M \lambda_\sigma^{M/2}$ occurs as a coefficient of the term on the right.

The poles of Equation (16) are somewhat more difficult to obtain, but perhaps a graphical procedure is the least difficult.

TABLE 2. SYSTEM ZEROS

ϕ	s_k
0.47	-1.16
1.10	-5.87
1.98	-15.03
2.35	-18.32

After substitution of the numerical values the denominator of Equation (16) is

$$c_s [c_s (\sin 6\theta - 0.59 \sin 5\theta) (\sin 5\phi - 0.724 \sin 4\phi) - 0.69 (\sin 5\theta - 0.59 \sin 4\theta) (\sin 5\phi - 0.724 \sin 4\phi) - (\sin 6\theta - 0.59 \sin 5\theta) (\sin 4\phi - 0.724 \sin 3\phi)] = 0 \quad (19)$$

The c_s outside the brackets cancels the c_s in the numerator of Equation (16). It is necessary to find the values of θ and ϕ which satisfy Equation (19) and then in turn the corresponding values of s . First find the zeros of each of the four terms in Equation (19) by the method just given for calculating the zeros of the complete equations. The equations to be solved are

$$\begin{aligned} \frac{\sin 5\theta}{\sin 4\theta} &= 0.59 & \frac{\sin 5\phi}{\sin 4\phi} &= 0.724 \\ \frac{\sin 6\theta}{\sin 5\theta} &= 0.59 & \frac{\sin 4\phi}{\sin 3\phi} &= 0.724 \end{aligned} \quad (20)$$

The values of ϕ for the third equation have already been given. Noting that $c_s = 0.186$ ($s + 10.75$) and upon substitution for the other roots one gets for Equation (19)

$$\begin{aligned} (s + 0.704) (s + 1.16) (s + 3.097) \\ (s + 5.87) (s + 7.10) (s + 10.70) \\ (s + 10.75) (s + 13.68) (s + 15.03) \\ (s + 18.34) - 13.9 (s + 1.05) \\ (s + 1.16) (s + 4.45) (s + 5.87) \\ (s + 9.09) (s + 13.17) (s + 15.03) \\ (s + 18.32) - 28.9 (s + 0.704) \\ (s + 1.817) (s + 3.097) (s + 7.10) \\ (s + 8.92) (s + 10.70) (s + 13.68) \\ (s + 18.14) = 0 \end{aligned} \quad (21)$$

The values of s satisfying Equation (21) can be found, although the process may be a little tedious. The graphical procedure involves plotting the sum of the two negative terms and the first term. The points of intersection are the values of s satisfying Equation (21). Since the zeros of each part are known, it is not difficult to find the approximate locations of the curves and to estimate the points of intersection. Then a few calculations will give the zeros of the complete equation. For columns with a large number of trays the process becomes very difficult. However it is relatively easy to set up the program for the determination of the zeros of Equation (21) on a digital computer. The final equation is

$$\bar{x}_a = \frac{840 (s + 1.16) (s + 5.87) (s + 15.03) (s + 18.32) \bar{x}_i}{(s + 0.360) (s + 0.905) (s + 2.50) (s + 4.20) (s + 6.80) (s + 9.50) (s + 11.80) (s + 13.80) (s + 17.80) (s + 18.80)} \quad (22)$$

Equation (22) is now a form from which it is not difficult to calculate the responses to any of several inputs. The response to a step input in the feed concentration is shown in Figure 5 and the frequency response curves in Figure 6.

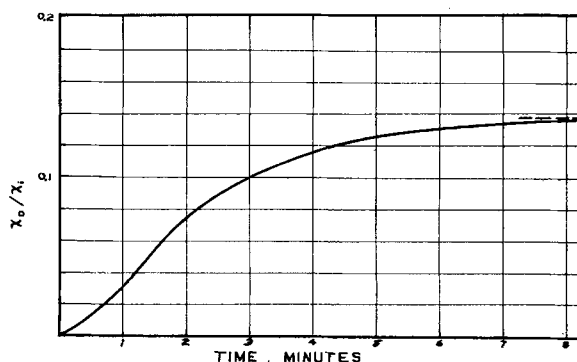


Fig. 5. Response to a step input.

The range of values covered by the poles and zeros in Equation (22) is quite large. The equation can be simplified, since poles which are more than ten times the smallest will have little effect upon the response to input changes. The poles of high value are effective at high frequencies only, but the amplitude ratio then is very small. Unfortunately there seems to be no easy method of calculating the significant poles without completing the calculation above.

PLATE EFFICIENCY

The tray efficiency was assumed to be 100% in the derivation of Equation (22). When the efficiency is not 100%, the general method can be used with the slopes of the equilibrium curve modified by

$$m = (1 - E) L/V + E m^* \\ m_s = \frac{(1 - E) (F + L)}{V} + E m_s^* \quad (23)$$

when m^* and m_s^* are the slopes when $E = 1$.

CONDENSER AND ACCUMULATOR CAPACITY

In the previous calculations the condenser liquid holdup was considered to be 0 in order to simplify the calculation. When the holdup is not 0, then certain modifications must be made in the equation. The equation for the top tray becomes

$$\bar{y}_n = \frac{\lambda \bar{y}_{n-1} - m \bar{x}_a}{c} \quad (24)$$

and for the condenser, when one assumes a first-order lag

$$\bar{x}_a = \frac{\lambda \bar{y}_n}{m(\alpha' s + D/L + 1)} = \frac{\lambda}{c'} \bar{y}_n \quad (25)$$

The signal flow diagram can be drawn, and the reduction of the diagram pro-

ceeds in the same manner as previously. The equation for the enriching section is now

$$\bar{x}_a = \frac{\lambda^{N+2} \sin \theta}{c' \sin(N+1)\theta - m\lambda^{1/2} \sin N\theta} \bar{y}_n \quad (26)$$

and the equation for the loop function H is

$$H = \frac{\lambda^{1/2} R [c' \sin N\theta - m\lambda^{1/2} \sin(N-1)\theta]}{c_s [c' \sin(N+1)\theta - m\lambda^{1/2} \sin N\theta]} \quad (27)$$

The problem of locating the poles of Equation (26) and the poles and zeros of Equation (27) is now slightly more difficult. For example in Equation (26) the poles correspond to values of θ which make the denominator 0. Now

$$s = \frac{2\lambda^{1/2} \cos \theta - 1 - \lambda}{\alpha}$$

and

$$c' = m\alpha's + \lambda = \frac{m\alpha' (2\lambda^{1/2} \cos \theta - 1 - \lambda)}{\alpha} + \lambda$$

Therefore the poles correspond to the values of θ which satisfy

$$\frac{\sin(N+1)\theta}{\sin N\theta} = \frac{m\lambda^{1/2} \alpha}{m\alpha' (2\lambda^{1/2} \cos \theta - 1 - \lambda) + \alpha \lambda} = \frac{m/\lambda^{1/2}}{\frac{m\alpha'}{\alpha \lambda} (2\lambda^{1/2} \cos \theta - 1 - \lambda) + 1} \quad (28)$$

These values of θ can be found by plotting the right side of the equation on the same graph as the left side. The points of intersection are the values of θ that satisfy Equation (28). This process can be simplified if $mC/L \cong \alpha$.

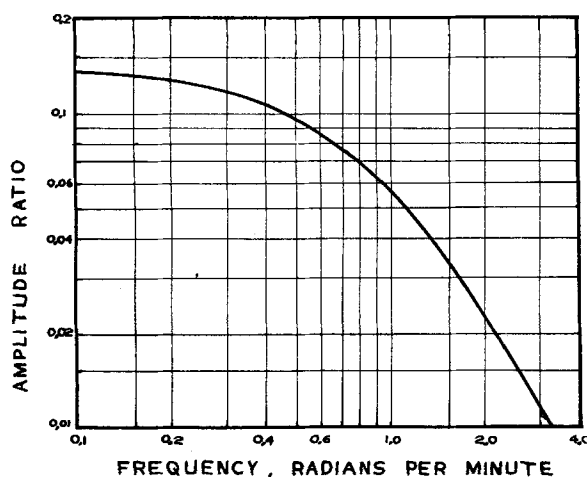


Fig. 6. Frequency response.

Similarly the equation for the bottom of the column can be written to take into account the capacitance of the reboiler if it is different from that of a tray. Unless the reboiler capacitance is very large, the effect on the response will be small.

CONCLUSIONS

Inspection of the equations and the signal flow diagrams reveals some interesting facts.

1. Equation (22) shows that the zeros and poles are all real and negative. Therefore the column is always stable and the transient responses are overdamped.

2. Figure 2d shows that between any two trays in the enriching section

$$y_n = \frac{K(s + z_1)(s + z_2) \dots (s + z_{N-n})}{(s + p_1)(s + p_2) \dots (s + p_{N+1-n})} y_{n-1}$$

3. From Figure 4a it is seen that the function for the enriching section has only poles equal in number to the number of trays above the feed tray.

4. The loop function H produced by the enriching section [Equation (13)] indicates that the function has $N-1$ zeros and $N+1$ poles.

5. The loop function U produced by the stripping section [Equation (15)] has $M-1$ zeros and $M+1$ poles. M includes the reboiler as a tray.

6. The complete equation for the column, that is Equations (16) or (22), has M zeros and $M+N+1$ poles.

7. The values of θ and ϕ corresponding to zeros or poles in the equation are primarily functions of the number of trays as can be seen from Equation (17). The constant in the equation, a function of V , L , and m , has little effect upon θ or ϕ .

8. The values of s_k corresponding to θ and ϕ are primarily functions of $\alpha = C/L$ and $\alpha_s = C/(F+L)$, as can be seen from Equation (18). That is the

tray capacitance and the liquid flow rates determine the magnitudes of s_k .

9. The values of the poles of the over-all function as shown in Equation (22) and determined from Equation (21) are difficult to relate directly to the column parameters.

10. The responses of the system are determined by the significant poles and zeros, that is those nearest the origin. Poles and zeros which are more than ten or more times as far from the origin as the closest ones will have little effect upon the responses. The result is that although the complete equation indicates a system of order $M+N+1$, the system can be satisfactorily represented by an equation of order 3 or 4.

11. The m which is used in the calculations is the slope of the equilibrium line and is a function of the tray efficiency. The effect of a change in the efficiency is negligible upon θ and ϕ , and as pointed out in item 8 above the effect upon s_k is also small.

12. The addition of a finite condenser lag or capacity can be included in the equations, but the calculation of the poles of Equation (26) and the poles and zeros of Equation (27) becomes somewhat more difficult. The equation for the column now has M zeros and $M+N+2$ poles.

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NOTATION

\bar{x}	= bar indicates transformed variable
A	= function as defined in paper
c	= $1 + \lambda + \alpha s$
c'	= $m\alpha' s + \lambda$
C	= tray capacitance

D	= product-molar flow rate
E	= tray efficiency
F	= feed-molar flow rate
G	= transfer function
H	= function as defined by Equation (13)
K	= constant
L	= liquid-molar flow rate
m	= slope of the vapor liquid equilibrium curve
M	= top tray of the stripping section and the feed tray = number of trays in the stripping section including the reboiler as a tray
N	= top tray of the enriching section = number of trays in the enriching section
p	= poles
R	= $m_s L / m(F + L)$
s	= independent variable in transformed equations
t	= time
U	= function as defined by Equation (15)
V	= vapor-molar flow rate
x	= change from the steady state in the liquid concentration
y	= change from steady state in the vapor concentration
z	= zeros

Greek Letters

α	= C/L
α'	= C_s/L
θ	= $\tan^{-1} \sqrt{4\lambda - c^2}/c$
λ	= Vm/L
λ_r	= $Fm_s/(F + L)$
ϕ	= $\tan^{-1} \sqrt{4\lambda_s c - c_s^2}/c_s$

Subscripts

1, 2, ...	= tray numbers, starting from the bottom
a	= accumulator
d	= product
m	= m th tray in the stripping section
n	= n th tray in the enriching section
σ	= stripping section

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