would be adiabatic or constant wall temperature in laminar flow. This is followed by isothermal or constant wall temperature in plug flow. Least desirable is an isothermal laminar flow reactor.

ACKNOWLEDGMENT

The authors wish to express their appreciation to the Marathon Oil Company for assistance in this work.

NOTATION

A = frequency factor, (liter/mole)$^{1/2}$/sec.
B = molar ratio of hydrogen to toluene
C = constant in Equation (12)
C_0, C_{H_2}, C_T = concentrations: initial, hydrogen, and toluene, respectively, g.-mole/cc.
C_P = specific heat of reaction mixture, cal./(g.-mole) (°K.)
D = diffusivity of toluene in reaction mixture, sq.cm./sec.
D_{TB}, D_{TC}, D_{TD} = binary diffusion coefficients with toluene as one of the components, sq.cm./sec.
E = activation energy, cal./g.-mole
$\Delta H°$ = heat of reaction, cal./g.-mole
k = thermal conductivity of reaction mixture, cal./(sec.)(cm.)(°K.)
L = reactor length, cm.
m = radial increment index
M = molar flux, g.-moles/(sec.)(sq.cm.)
MW = molecular weight, g./g.-mole
Q = rate of heat transfer, cal./(cc.)(sec.)
r = radial distance from center line, cm.
R = reactor radius, cm.
R^* = reaction rate, g.-mole/(cc.)(sec.)
T = temperature, °K.
T_0 = inlet temperature, °K.
u = point velocity, cm./sec.
V = center-line velocity, cm./sec.
x = conversion of toluene
y_T, y_B ... = mole fraction of toluene, component B, etc.
z = axial distance from reactor inlet, cm.
μ = viscosity, poise
θ = time, sec.

Subscripts

m = radial increment index
mix = mixture
n = axial increment index
ref = reference conditions

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Distillation Decoupling

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This paper presents a quantitative study of two types of decoupling elements to achieve noninteracting feedback control of overhead and bottoms compositions in binary distillation. Ideal decoupling, where the closed loop response of each loop is the same as it would be if the other loop were on manual control, and simplified decoupling, where two interaction compensators are used to isolate each loop, are investigated.

The decoupling elements themselves are physically realizable in both cases, but unstable loops develop with ideal decoupling in higher purity columns because of increased positive feedback. Simplified decoupling gave effective, stable, noninteracting loops for all the cases studied.

The decoupling elements are designed in the frequency domain from a linear model of the column, and their effectiveness is tested by digital simulation of the nonlinear column model.

Distillation columns continue to represent major control problems in many industries. The complex, multistage nature of distillation columns requires proficiency in the fundamentals of operation, both steady state and dynamic, plus experience to successfully analyze and diagnose their operation.

Of all the distillation column control problems, one of the most important and controversial, and still unresolved, is the control of product compositions at both ends of the column. The usual control system on an industrial column attempts to hold the composition constant at only one end of the column or on some suitable control tray. The composition at the other end then varies with any change in conditions. The end chosen to be controlled is presumably the more important one, from some standpoint.

However, purities of the overhead product and the bottoms product are frequently both important. Composition fluctuations in either end can cause upsets in subsequent process units and lead to costly off-specification products. There are several brute force techniques that are routinely used to circumvent this problem, but all involve significant increases in operating or capital costs:

1. Build columns with many more trays than are required for normal operation so that the purity of the wild stream will be good enough even under the most adverse conditions.
2. Run columns at higher reflux ratios than are required for normal operation.
3. Build large feed tanks to attenuate feed disturbances or build large product tanks to blend off-specification material.
4. Build cleanup columns on product streams.

Control problems have often been experienced when feedback control of both product compositions has been attempted. There are undoubtedly many reasons for control instabilities and poor performance (for example, reversals in control action due to nonlinearities: reference *3*), but one of the principle difficulties is control loop interaction. Changes in vapor boil up V_B to control bottoms composition X_B also affect overhead composition X_D. Likewise, changes in reflux flow R to control X_D disturb X_B. Figure 1*a* shows a coupled system in general matrix form and specifically for the two-dimensional distillation example.

Several discussions of interaction in distillation column control have appeared in the literature. Rosenbrock (*7*) was one of the first to point out that little work had been directed toward the interaction problem. He illustrated some of the detrimental effects of interaction by analogue simulation of an arbitrary linear system. Rosenbrock also proposed a unique control system to reduce the interaction by controlling the sum and the difference of two internal compositions by reflux and vapor boil up, respectively.

Rijnsdorp (*5, 6*) proposed a ratio control scheme between reflux and top vapor flow to reduce interaction effects. Buckley (*1*) has suggested the simple and intuitively appealing scheme of inserting two interaction compensators, much like feedforward controllers, to cancel out the effects of each manipulative variable on the composition at the opposite end of the column.

The purpose of this paper is to study the design and performance of Buckley's simplified decouplers and an ideal decoupler for several binary distillation columns. The approach is to synthesize the decoupling elements in the frequency domain from a linear model of the column and then to test their effectiveness on the nonlinear system by digital simulation.

LINEAR COLUMN MODEL

The open loop plant transfer functions of the linear model of the column **P** and $\mathbf{P}^m$ between outputs and disturbances and outputs and manipulative variables were found by using the frequency domain solution technique (*2*). Equations, assumptions, steady state conditions, and coefficients of the linear differential equations are given in reference *4*:

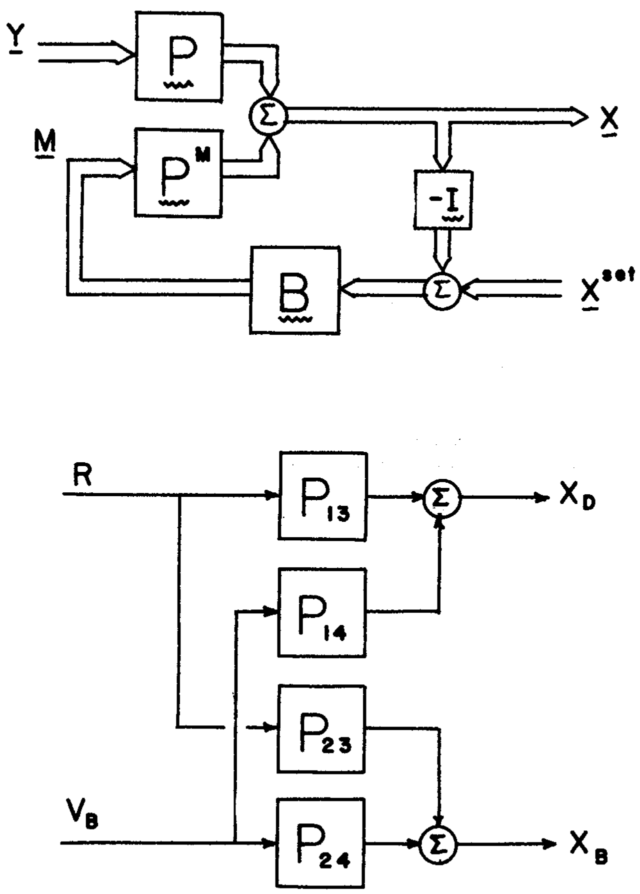

Fig. 1*a*. Block diagram coupled system.

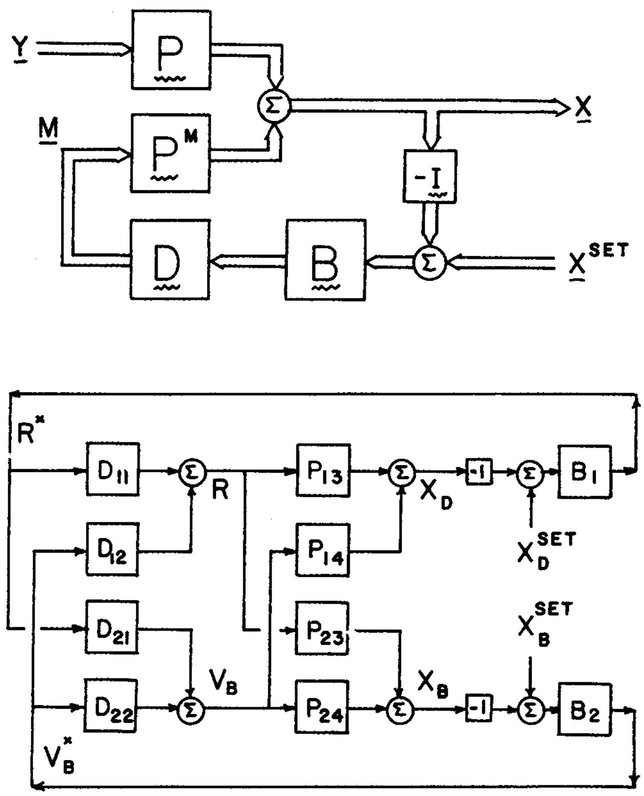

Fig. 1*b*. Block diagram ideal decoupling.

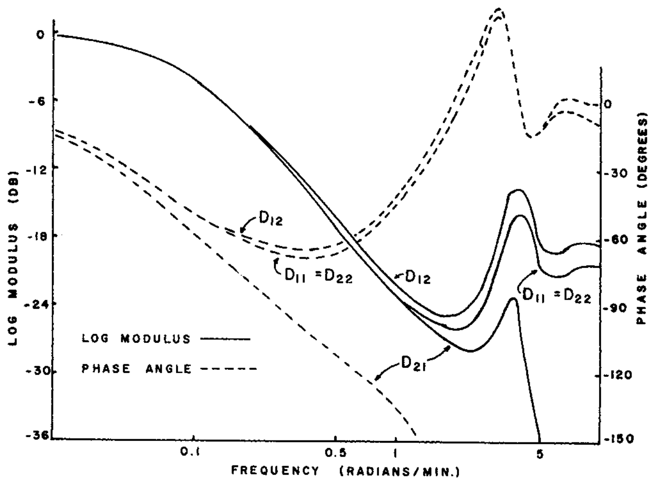

Fig. 2a. Bode plots of ideal decouplers (2/98 case).

$$X = \mathbf{P}\,\underline{Y} + \mathbf{P}^m\,\underline{M} \tag{1}$$

For the two-dimensional distillation example, the equations are

$$\begin{bmatrix} X_D \\ X_B \end{bmatrix} = \begin{bmatrix} P_{11}\,P_{12} \\ P_{21}\,P_{22} \end{bmatrix}\begin{bmatrix} X_F \\ F_L \end{bmatrix} + \begin{bmatrix} P_{13}\,P_{14} \\ P_{23}\,P_{24} \end{bmatrix}\begin{bmatrix} R \\ V_B \end{bmatrix} \tag{2}$$

With feedback controllers at each end of the column, manipulative variables $\underline{M}$ are related to outputs and set points:

$$M = \mathbf{B}\,(\underline{X}^{\text{set}} - \underline{X}) \tag{3}$$

$$\begin{bmatrix} R \\ V_B \end{bmatrix} = \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}\begin{bmatrix} X_D{}^{\text{set}} - X_D \\ X_B{}^{\text{set}} - X_B \end{bmatrix} \tag{4}$$

The closed loop matrix block diagram is given in Figure 1*a*. The closed loop response of the system is

$$\underline{X} = [\mathbf{I} + \mathbf{P}^m\,\mathbf{B}]^{-1}\,\mathbf{P}\,\underline{Y} + [\mathbf{I} + \mathbf{P}^m\,\mathbf{B}]^{-1}\,\mathbf{P}^m\,\mathbf{B}\,\underline{X}^{\text{set}} \tag{5}$$

IDEAL DECOUPLING

To eliminate the interaction between control loops, decoupling elements can be added, as shown in Figure 1*b*, giving a closed loop equation:

$$\begin{aligned} \underline{X} &= [\mathbf{I} + \mathbf{P}^m\,\mathbf{D}\,\mathbf{B}]^{-1}\,\mathbf{P}\,\underline{Y} + [\mathbf{I} + \mathbf{P}^m\,\mathbf{D}\,\mathbf{B}]^{-1}\,\mathbf{P}^m\,\mathbf{D}\,\mathbf{B}\,\underline{X}^{\text{set}} \\ &= \mathbf{K}_1\,\underline{Y} + \mathbf{K}_2\,\underline{X}^{\text{set}} \end{aligned} \tag{6}$$

For noninteracting control, the $\mathbf{K}_2$ closed loop transfer

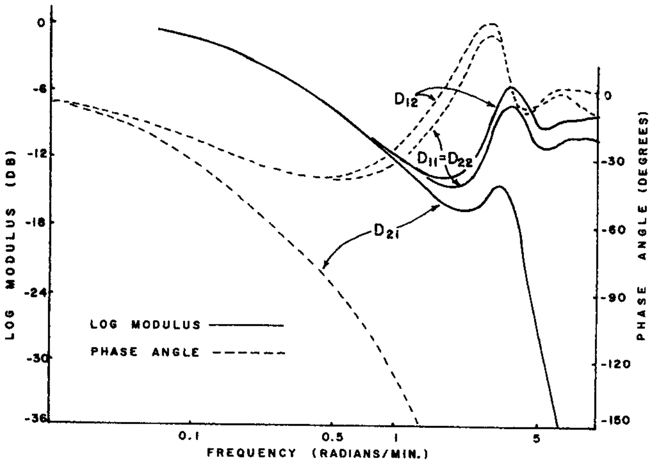

Fig. 2b. Bode plots of ideal decouplers (5/95 case).

function matrix must be diagonal and, of course, must be specified.

The intuitive first choice of the distillation control engineer might be to want each loop to behave as if the other were not on control. That is, the response of each loop (with both on automatic control) should be the same as the response one would get if the other loop were on manual (thus fixing the other manipulative variable). For example, if the top loop is on automatic and vapor boil up is constant, the response of X_D is given by

$$X_D = \left[\frac{P_{11}}{1 + B_1P_{13}}\right] X_F + \left[\frac{P_{12}}{1 + B_1P_{13}}\right] F_L + \left[\frac{B_1P_{13}}{1 + B_1P_{13}}\right] X_D{}^{\text{set}} \tag{7}$$

Likewise, the response of X_B with only the bottom loop on control and reflux fixed would be

$$X_B = \left[\frac{P_{21}}{1 + B_2P_{24}}\right] X_F + \left[\frac{P_{22}}{1 + B_2P_{24}}\right] F_L + \left[\frac{B_2P_{24}}{1 + B_2P_{24}}\right] X_B{}^{\text{set}} \tag{8}$$

We shall define these two responses as ideal and specify the closed loop transfer matrix $\mathbf{K}_2$ to give the responses shown in Equations (7) and (8) with both loops on automatic control. Therefore

$$\mathbf{K}_2 = \begin{vmatrix} \left(\frac{B_1P_{13}}{1 + B_1P_{13}}\right) & 0 \\ 0 & \left(\frac{B_2P_{24}}{1 + B_2P_{24}}\right) \end{vmatrix} \tag{9}$$

$$[\mathbf{I} + \mathbf{P}^m\mathbf{D}\mathbf{B}]^{-1}\,\mathbf{P}^m\mathbf{D}\mathbf{B} = \begin{vmatrix} \left(\frac{1}{1 + B_1P_{13}}\right) & 0 \\ 0 & \left(\frac{1}{1 + B_2P_{24}}\right) \end{vmatrix} \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}\begin{bmatrix} P_{13} & 0 \\ 0 & P_{24} \end{bmatrix}$$

The above requires that

$$\mathbf{P}^m\,\mathbf{D} = \begin{bmatrix} P_{13} & 0 \\ 0 & P_{24} \end{bmatrix} \equiv [\text{Diag}\,P^m] \tag{10}$$

Thus, the design equation for the decoupling elements to achieve ideal noninteracting control is

$$\mathbf{D} = [\mathbf{P}^m]^{-1}\,[\text{Diag}\,P^m] \tag{11}$$

Or, for the distillation example

$$\begin{vmatrix} D_{11}\,D_{12} \\ D_{21}\,D_{22} \end{vmatrix} = \begin{vmatrix} \left(\frac{P_{13}P_{14}}{P_{13}P_{24} - P_{14}P_{23}}\right) & \left(\frac{-P_{14}P_{24}}{P_{13}P_{24} - P_{14}P_{23}}\right) \\ \left(\frac{-P_{13}P_{23}}{P_{13}P_{24} - P_{14}P_{23}}\right) & \left(\frac{P_{13}P_{14}}{P_{13}P_{24} - P_{14}P_{23}}\right) \end{vmatrix} \tag{12}$$

Ideal decouplers for several distillation columns were

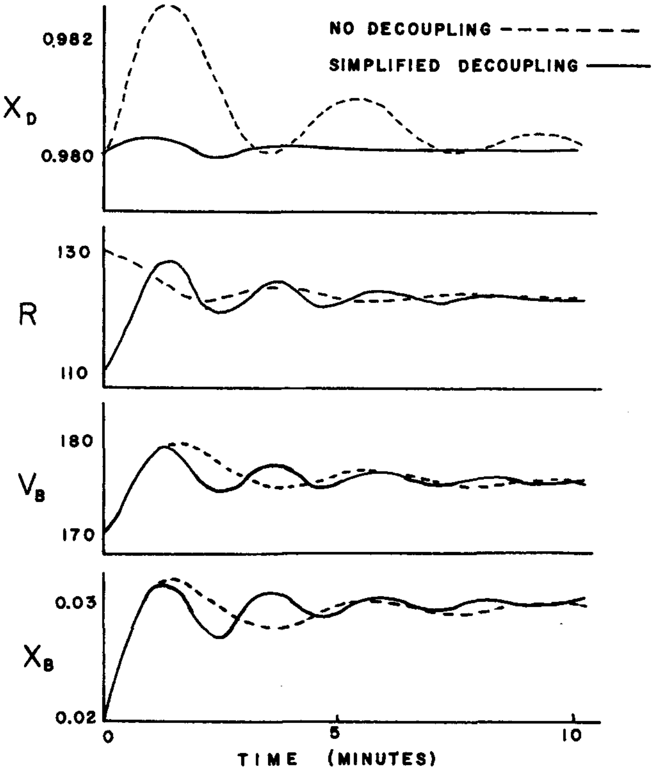

Fig. 3a. Transient response (2/98 case) with X_D^{set} disturbance.

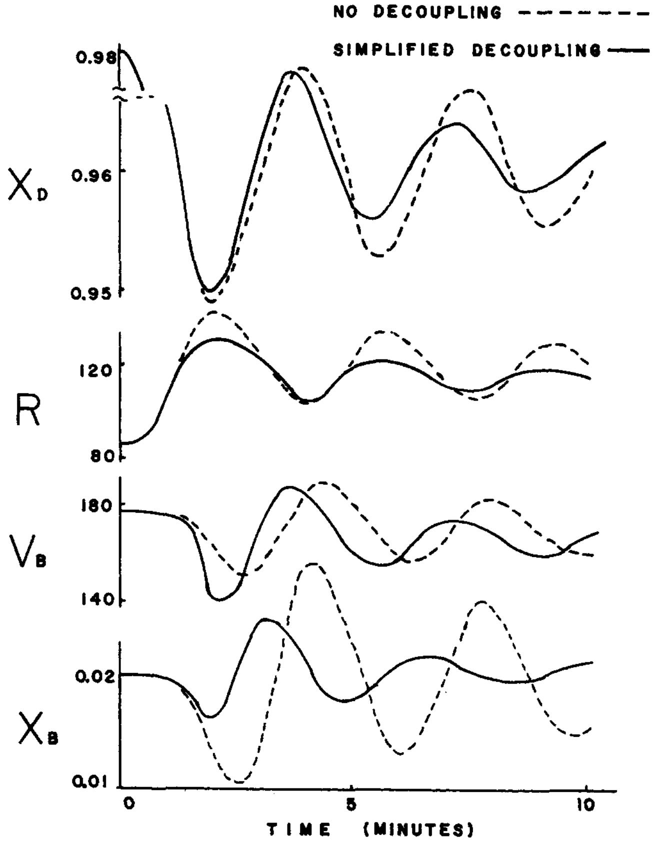

Fig. 3b. Transient response (2/98 case) with X_D^{set} disturbance.

calculated. Table 1 gives steady state gains for these decoupling elements. Note the rapid increase in gain as product purities increase. Figures 2*a* and 2*b* give Bode plots for two cases: $X_D = 0.95$ and $X_B = 0.05$, and $X_D = 0.98$ and $X_B = 0.02$. The decoupling elements are physically realizable.

Approximate transfer functions were fitted to the Bode plots by using first- and second-order lags and lead-lag networks:

	2/98 case	5/95 case
$D_{11} = D_{22}$	$\dfrac{10.62}{12.5\,s + 1}$	$3.298\left[\dfrac{1.5\,s + 1}{5\,s + 1}\right]$
D_{12}	$\dfrac{10.08}{12.5\,s + 1}$	$2.697\left[\dfrac{1.5\,s + 1}{5\,s + 1}\right]$
D_{21}	$\dfrac{10.14}{12.5\,s + 1}$	$\dfrac{2.809}{(2\,s + 1)^2}$

A two-mode feedback controller was used for all cases with gain $K_c = 2{,}000$ and reset $\tau_i = 2$ min.:

$$B_{(s)} = K_c\left(1 + \frac{1}{\tau_i\, s}\right) \qquad (13)$$

Table 1. Steady State Gains of Ideal Decoupling Elements

X_B	X_D	F_L	X_F	Steady state gains D_{11}	D_{12}	D_{21}	Reflux	ω_{-3db} *
0.05	0.95	100	0.50	3.30	2.70	2.81	146	0.18
0.02	0.98	100	0.50	10.62	10.08	10.14	128	0.08
0.01	0.99	100	0.50	33.80	33.28	33.31	165	0.045
0.005	0.995	100	0.50	126.74	126.24	126.23	230	0.025
0.02	0.98	60	0.50	10.62	10.08	10.14	76.8	0.05
0.02	0.98	140	0.50	10.62	10.08	10.14	179	0.11
0.02	0.98	100	0.60	10.86	10.37	10.33	125	0.08
0.02	0.98	100	0.40	10.69	10.11	10.25	128	0.08

* Where log modulus = $-3db$.

Results of the digital simulation of the nonlinear equations describing the column with feedback controllers and decouplers are given in Figures 3*a* to 3*d*. The nonlinear model included a nonlinear vapor/liquid equilibrium relationship (constant relative volatility) and variable tray holdups. Numerical values of parameters and steady state conditions are given in reference *4*.

The system was found to be unstable for the 2/98 case but stable for the 5/95 case. The reason for the onset of instability as product purities increase is the positive feedback that the decouplers introduce into the system. The higher the purities, the larger the positive feedback effect becomes, because the decoupler gains increase (see Table 1).

Thus, it appears that ideal decoupling may be of limited applicability. This scheme would also require four dynamic elements. There are, of course, other reasons for the onset of instability: nonlinearity of the system and inaccuracies in approximating the decoupling element Bode plots. Better approximation should extend the range of stability, but the fits were purposely made fairly rough in this study to test the sensitivity of performance to modeling accuracy.

SIMPLIFIED DECOUPLING

Buckley (*1*) has suggested that a particularly simple way to decouple overhead and bottoms feedback loops would be to insert two interaction compensators that cancel the direct effect of one manipulative variable on a product composition by the correct change in the other manipulative variable.

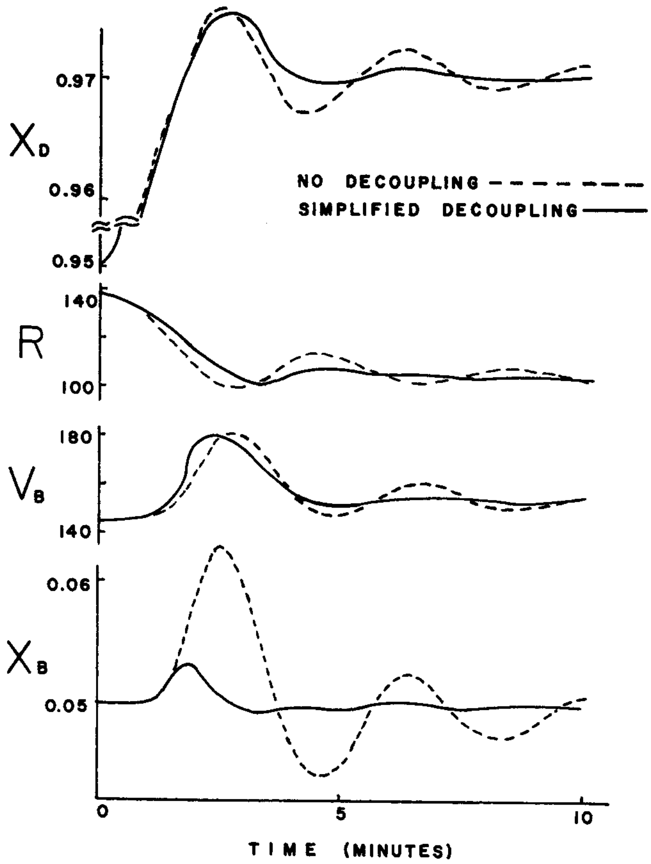

Fig. 3c. Transient response (5/95 case) with X_B^{set} disturbance.

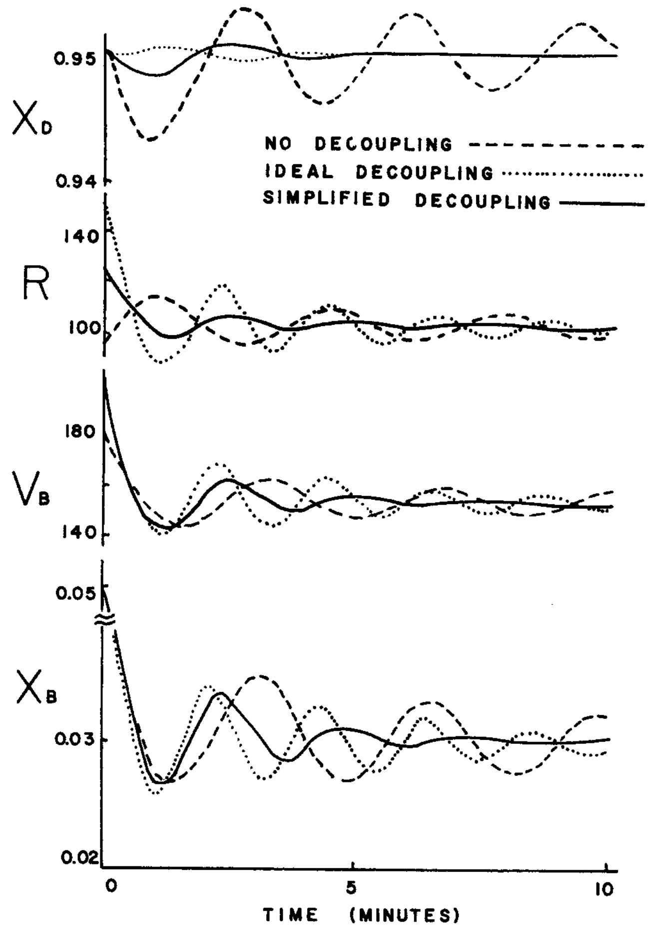

Fig. 3*d*. Transient response (5/95 case) with X_B^{set} disturbance.

Consider the effects of both manipulative variables on only X_D:

$$X_D = P_{13}\,R + P_{14}\,V_B$$

Suppose X_D is exactly what it should be, that is, equal to X_D^{set}, and the bottom controller changes V_B because of a disturbance in the base of the column. This change in V_B will upset X_D too, if no other action is taken. If, however, we change the reflux R to cancel out the effect of V_B on X_D, the top loop will be undisturbed. In a sense we are using feedforward control inside the feedback loops. Note that the change in R will affect the bottom loop, giving a different closed loop response for X_B than without decoupling.

Thus, we want overhead composition to be held constant, that is, X_D held equal to zero, since it is a perturbation variable:

$$X_D = 0 = P_{13}\,R + P_{14}\,V_B$$

$$\frac{R}{V_B} = \frac{-P_{14}}{P_{13}} \equiv D_{2(s)} \tag{14}$$

The decoupling element D_2 is the interaction compensator between R and V_B.

Similar arguments for the control of X_B yield

$$\frac{V_B}{R} = \frac{-P_{23}}{P_{24}} \equiv D_{1(s)} \tag{15}$$

Equations (14) and (15) are the design equations for the simplified decoupling elements. Block diagrams for this system are shown in Figure 4. Only two dynamic elements are needed.

The closed loop response of the system will not be the same as with ideal decoupling. With ideal decoupling, the closed loop characteristic equations (CLCE) for the two loops are

$$\begin{array}{ll} \text{Top CLCE:} & 1 + B_1\,P_{13} \\ \text{Bottom CLCE:} & 1 + B_2\,P_{24} \end{array} \tag{16}$$

With simplified decoupling, the closed loop characteristic equations are

$$\text{Top CLCE:} \quad 1 + B_1\left[\frac{P_{13}P_{24} - P_{14}P_{23}}{P_{24}}\right] = 1 + B_1\,G_{c1}$$

$$\text{Bottom CLCE:} \quad 1 + B_2\left[\frac{P_{13}P_{24} - P_{14}P_{23}}{P_{13}}\right] = 1 + B_2\,G_{c2}$$

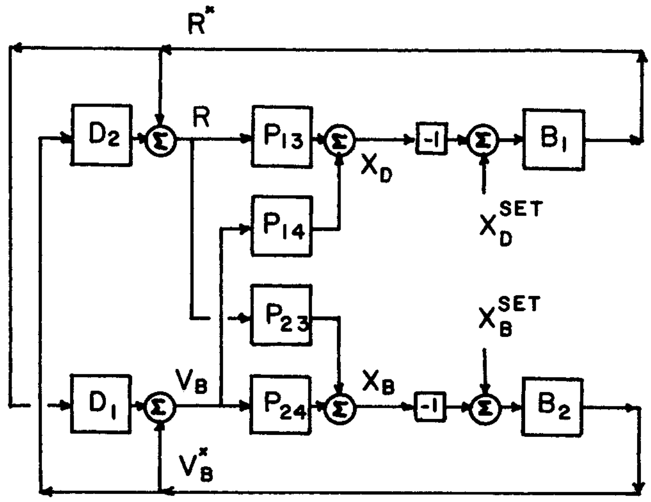

Fig. 4. Block diagram simplified decoupling.

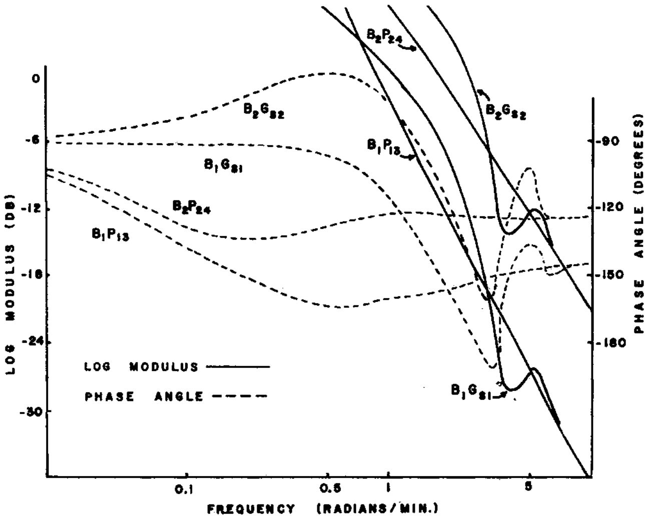

Fig. 5. Open loop frequency response of feedback loops with ideal and simplified decoupling.

Bode plots for the B_iP_i and B_iG_{ci} are compared in Figure 5 with the 2/98 case with $K_c = 2{,}000$ and $\tau_i = 2$ min.

Table 2 gives steady state gains of the simplified decouplers for several cases. Notice that the gains, instead of becoming larger as product purities increase, approach a limit of one. Bode plots are given in Figure 6. Results for the 2/98 and 5/95 cases were practically identical. The D_2 transfer function is a simple constant. The D_1 transfer function was represented by a first-order lag with dead time:

	2/98 case	5/95 case
D_1	$\dfrac{0.9547\,e^{-1.5s}}{0.4\,s+1}$	$\dfrac{0.8518\,e^{-1.5s}}{0.4\,s+1}$
D_2	0.9488	0.8180

The effectiveness of the simplified decouplers on the nonlinear column is shown in Figures 3*a* to 3*d*. Performance is excellent in all the cases studied.

CONCLUSIONS

Decoupling elements can be designed from a linear model of distillation columns. Two types of decouplers, ideal and simplified, were both physically realizable. Positive feedback increases with product purities in ideal decoupling, leading to unstable feedback loops. Simplified decoupling is effective and stable and appears to be easily implemented with commercial control instrumentation.

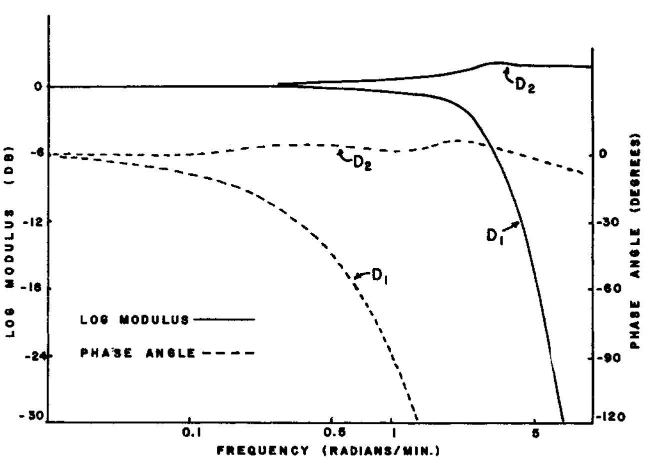

Fig. 6. Bode plots of simplified decouplers.

TABLE 2. STEADY STATE GAINS OF SIMPLIFIED DECOUPLING ELEMENTS

X_B	X_D	X_F	D_1	D_2
0.05	0.95	0.50	0.8518	0.8180
0.02	0.98	0.50	0.9547	0.9488
0.01	0.99	0.50	0.9856	0.9846
0.005	0.995	0.50	0.9960	0.9961

NOTATION

$\mathbf{B}$ = feedback controller matrix
B_1 = feedback controller on overhead composition loop
B_2 = feedback controller on bottoms composition loop
$\mathbf{D}$ = matrix of decoupling elements
D_1 = simplified decoupler in base of column $-V_B/R$
D_2 = simplified decoupler in top of column $-R/V_B$
D_{ij} = ideal decoupling elements
$[\text{Diag}\, P^m]$ = diagonal matrix formed from the diagonal elements of the P^m matrix
F_L = feed flow rate, moles/min.
G_{ci} = equivalent open loop transfer functions with simplified decoupling
$\mathbf{I}$ = identity matrix
$\mathbf{K}_1$ = matrix of closed loop transfer functions relating outputs to disturbances
$\mathbf{K}_2$ = matrix of closed loop transfer functions relating outputs to set points
$\underline{M}$ = manipulative variables
$\mathbf{P}$ = matrix of open loop transfer functions relating outputs to disturbances
$\mathbf{P}^m$ = matrix of open loop transfer functions relating outputs to manipulative variables
R = reflux flow rate, moles/min.
V_B = vapor boil up rate, moles/min.
$\underline{X}$ = output variables
$\underline{X}^{set}$ = set point variables
X_B = bottoms composition, mole fraction
X_F = feed composition, mole fraction
X_D = distillate overhead composition, mole fraction
$\underline{Y}$ = disturbance variables
K_c = feedback controller gain, moles/min.
τ_i = feedback controller reset time, min.

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