nitrogen oxides to be present in the form of N_2O_4. Consequently, higher plate efficiencies may be obtained by increasing the total pressure of the gases.

The experimental data obtained with the bubble-cap column showed that an increase in the gas rate caused a decrease in the fraction of entering oxides converted to nitric acid, but a twofold change in the liquid-flow rate had no appreciable effect on the fractional conversion.

SUMMARY

The factor which controls the over-all mechanism in the removal of nitrogen oxides from gaseous mixtures by contact with water is the rate of the chemical reactions involved. The rate of removal of the nitrogen oxides is proportional to the concentration of N_2O_4 in the gases. As the fraction of total oxides present as N_2O_4 is low when the concentration of gaseous oxides is low, the individual plate efficiencies for removal of nitrogen oxides from dilute gases are poor; however improved plate efficiencies can result with high total pressure.

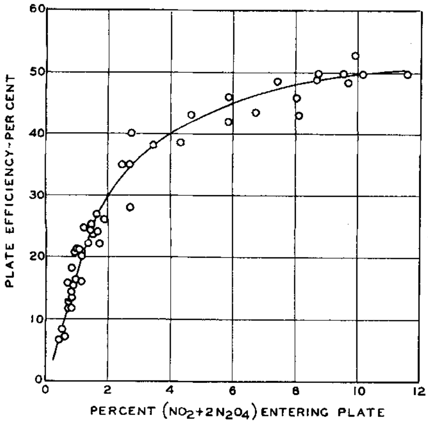

FIG. 4. EFFECT OF eNO_2 CONCENTRATION IN ENTERING GASES ON ABSORPTION EFFICIENCY (BUBBLE-CAP COLUMN AT 1 ATM. TOTAL PRESSURE; GAS-SLOT VELOCITY OF 1.18 FT./SEC.)

The chemical reactions between nitrogen oxides and water occur partially in the gas phase or in the gas film, as evinced by the formation of a mist when NO_2 and N_2O_4 are in vapor.

The fraction of the entering oxides which are converted to nitric acid decreases as the contact time between the gas and liquid decreases. If experimental data for the equipment are available at one gas rate, the integrated kinetic equations can be used for an estimation of the effect of change in gas-liquid contact time.

ACKNOWLEDGMENT

This work has been conducted in the Engineering Experiment Station of the University of Illinois as part of Contract AT(30-3)-28, United States Atomic Energy Commission, H. F. Johnstone, technical director. Detailed information concerning the theory and experimental results are available as Technical Report 10, COO-1011, Technical Information Service, United States Atomic Energy Commission, Oak Ridge, Tennessee.

NOTATION

A = constant at any temperature
B = constant at any temperature
C = concentration, gram moles/cc.
C_f = final concentration, gram moles/cc.
C_o = original concentration, gram moles/cc.
D = diffusivity, sq. cm./sec.
eNO_2 = equivalent $NO_2 = NO_2 + 2\ N_2O_4$
k = reaction-rate constant, units depending on reaction involved
K = equilibrium constant for the reaction, $2\ NO_2 = N_2O_4$
N_{eNO_2} = rate of nitrogen oxides removal based on equivalent NO_2 removal, gram moles/(sec.) (sq. cm.)
P = partial pressure, atm.
P_f = final partial pressure, atm.
P_o = original partial pressure, atm.
t = time, sec.
x_f = effective film thickness, cm.
ΔC = differences in concentration between main body of gas and gas-liquid interface, gram moles/cc.

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(Presented at A.I.Ch.E. Washington meeting)

APPROXIMATE EQUATIONS FOR TIME OF BATCH FRACTIONATION

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Analytical expressions are obtained for the calculation of the time required for batch rectification of binary feeds which may be treated by assuming constant relative volatility and no column holdup. The equations cover constant reflux operations and varying reflux constant product operations for the two cases involving either a large or a small number of theoretical stages. The latter type of calculation has hitherto been possible only by tedious graphical methods. This paper introduces novel pseudo-equilibrium curves which lead to simple equations of considerable accuracy. The equations obtained may be rearranged or modified so that other factors such as sharpness of fractionation may be represented analytically.

An accurate method for the design of equipment for the batch distillation and fractionation of binary liquid mixtures of constant overhead product composition with varying reflux ratio was presented by Bogart(*1*). However, the method covered only the case of constant distillate composition with varying reflux ratio and involved a rather tedious graphical integration. Many subsequent papers have dealt with modifications of assumptions made by Bogart, notably the inclusion of the effect of holdup.

These papers are summarized in a recent excellent paper by Rose and Johnson(*5*), who also list all the variables which must be considered in any accurate computation method.

Another recent paper which is relevant to the present work is that of Chu(*2*). Analytical expressions are derived for calculating the yield of distillate obtainable in a batch distillation carried out with increasing reflux to a predetermined value.

The present paper discusses approximate analytical methods for constant-reflux and constant-overhead-composition batch distillations for binary systems with constant relative volatility. The equations derived permit the calculation of the time required, θ, to reduce the initial composition in the pot, x mole fraction more volatile, to a final composition x mole fraction in an apparatus containing n theoretical plates.

Depending on the number of plates, two situations arise. When n is large, the intersection of the operating line and equilibrium curve is usually at the same composition abscissa as is the pot composition for all practical purposes. The equations for θ may be derived easily, as outlined. However, when n is small, this assumption is considerably in error. For this case pseudoequilibrium curves are developed leading to equations for θ.

In addition to constant relative volatility all the usual simplifying assumptions made in applying the McCabe-Thiele method are employed: ideal plates, constant molal vaporization and overflow in the column at any instant, and an adiabatic column. The equations neglect holdup of liquid and vapor in the column and condenser.

DERIVATION OF EQUATIONS

Batch Operation Including a Large Number of Theoretical Plates. *Constant Reflux Ratio.* For constant relative volatility of α, the equation of the equilibrium curve is

$$y = \frac{\alpha x}{1 + (\alpha - 1)x} \qquad (1)$$

As the number of theoretical stages is large, the intersection of the operating line

$$y = \frac{R}{R+1}x + \frac{1}{R+1}x_{\mathrm{D}} \qquad (2)$$

and the equilibrium curve [Equation (1)] is for all practical purposes at the same composition abscissa as is the pot-liquid composition (*see* Figure 1). Eliminating y between Equations (1) and (2) gives the corresponding distillate composition, obtained as a function of pot-liquid composition x,

$$x_{\mathrm{D}} = \frac{\dfrac{\alpha x}{1 + (\alpha-1)x} - \dfrac{R}{R+1}x}{\dfrac{1}{R+1}} \qquad (3)$$

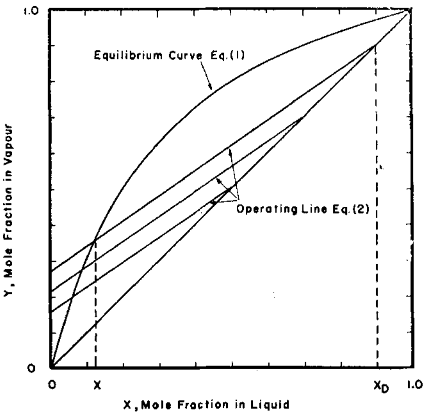

FIG. 1. CASE 1*a*, BATCH FRACTIONATION WITH CONSTANT REFLUX RATIO —LARGE NUMBER OF PLATES.

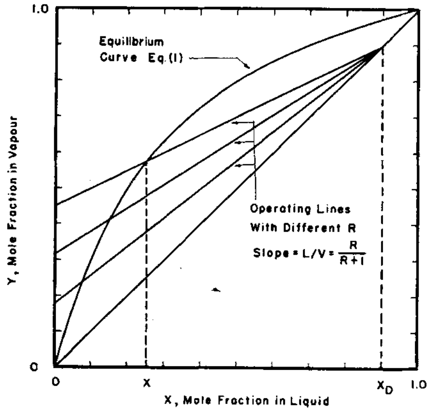

FIG. 2. CASE 1*b*, BATCH FRACTIONATION PRODUCING CONSTANT COMPOSITION OF DISTILLATE—LARGE NUMBER OF PLATES.

When this is substituted in the basic Rayleigh equation (4) or batch distillation,

$$\int_{W}^{W_i} \frac{dW}{W} = \int_{x}^{x_i} \frac{dx}{x_{\mathrm{D}} - x} \qquad (4)$$

and integrated,

$$\frac{W_i}{W} = \left[\frac{\dfrac{(1-x_i)^{\alpha}}{x_i}}{\dfrac{(1-x)^{\alpha}}{x}}\right]^{-\frac{1}{(\alpha-1)}\frac{1}{(R+1)}} \qquad (5)$$

This equation gives the relationship between the initial and final number of moles in the pot W_i and W and the initial and final pot-liquid compositions x_i and x. If the vaporizing rate is V moles/hr., the time required for this operation is

$$\theta = (R+1)\frac{W_i}{V}\Bigg\} 1 - \left[\frac{\dfrac{(1-x_i)^{\alpha}}{x_i}}{\dfrac{(1-x)^{\alpha}}{x}}\right]^{\frac{1}{(\alpha-1)}\frac{1}{(R+1)}}\Bigg\{ \qquad (6)$$

Variable Reflux Ratios, Producing Distillate of Constant Composition. For this case as the distillation proceeds, the reflux ratio must be increased to maintain a given product purity x_D, which is held constant. If the initial pot-liquid composition is x_i, the initial value of L/V (and therefore the initial reflux ratio) is obtained from Equation (3) by substitution of x_i for x. The initial reflux ratio required is

$$R_i = \frac{x_{\mathrm{D}} + (\alpha-1)\ x_i\ x_{\mathrm{D}} - \alpha x_i}{(\alpha-1)\ x_i\ (1-x_i)} \qquad (7)$$

The total time for any binary distillation producing distillate of constant composition has been developed by Bogart(*1*):

$$\theta = \frac{W_i\,(x_{\mathrm{D}} - x_i)}{V} \int_{x}^{x_i} \frac{dx}{(1 - \frac{L}{V})\ (x_{\mathrm{D}} - x)^2} \qquad (8)$$

The slope of the operating line (*see* Figure 2) may be expressed as

$$\frac{L}{V} = \frac{x_{\mathrm{D}} - y}{x_{\mathrm{D}} - x} \qquad (9)$$

and imposing constant relative volatility from Equation (1) enables Bogart's equation [Equation (8)] to be integrated to

$$\theta = \frac{W_i\,(x_{\mathrm{D}} - x_i)}{V(\alpha - 1)\,x_{\mathrm{D}}\ (1 - x_{\mathrm{D}})}$$

$$\Bigg\{ (1 - x_{\mathrm{D}}) \ln\frac{x_i}{x} + [1 + (\alpha-1)x_{\mathrm{D}}]$$

$$\ln \frac{x_D - x}{x_D - x_i} + \alpha x_D \ln \frac{1 - x_i}{1 - x} \Big\} \quad (10)$$

Batch Operation Involving a Small Number of Theoretical Plates. *Constant Reflux Ratio.* The proposed method for calculation involving a small number of theoretical plates and constant reflux ratio is based on the use of a pseudoequilibrium curve and the application of the method previously described.

The pseudoequilibrium curve is to relate pot composition and overhead composition for constant-reflux-ratio distillation. Furthermore, it should reflect the relative volatility of the system, the number of theoretical plates in the column, and the reflux ratio. A curve which does this with sufficient accuracy for engineering calculations may be developed as follows (*see* Figure 3).

Following is a consideration of the geometry corresponding to $x = 0.5$. This abscissa was chosen as a starting point because of the simple value of the ordinate, $y = \frac{\alpha}{\alpha + 1}$, on the true equilibrium curve *BEGD.* For the true equilibrium curve the pseudoline *FD* is substituted. This line also has a rather simple equation

$$y = \frac{2}{\alpha + 1} x + \frac{\alpha - 1}{\alpha + 1} \quad (11)$$

or

$$y = m_2 x + b_2 \text{ where } m_2 =$$

$$\frac{2}{\alpha + 1} \text{ and } b_2 = \frac{\alpha - 1}{\alpha + 1} \quad (12)$$

The equation of the operating line corresponding to the fixed reflux ratio and to the pot-liquid composition $x_n = 0.5$ may be

$$y = m_1 x + b_1 \quad (13)$$

where $m_1 = \frac{R}{R + 1}$

$$b_1 = \frac{x_D}{R + 1}$$

A relationship between x_n and x_D can be developed by a method similar to that of Smoker(7). Corresponding to $x_n = 0.5$, the composition of equilibrium vapor is $\alpha / (\alpha + 1)$.

From Equation (13),

$$x_{n-1} = \frac{y_n - b_1}{m_1} = \frac{\frac{\alpha}{\alpha + 1} - b_1}{m_1} \quad (14)$$

By substitution in Equation (12),

$$y_{n-1} = m_2 \, x_{n-1} + b_2 =$$

$$\frac{m_2}{m_1} \left(\frac{\alpha}{\alpha + 1} - b_1\right) + b_2 \quad (15)$$

When this operation is continued from plate to plate and $r = \frac{m_2}{m_1}$

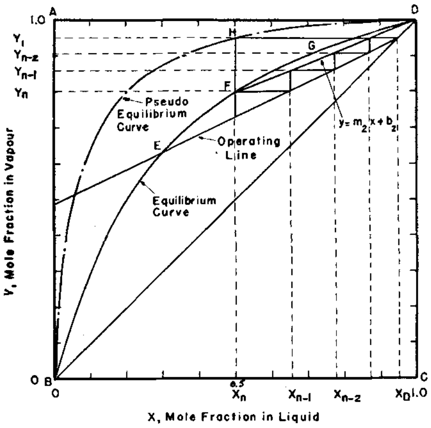

FIG. 3. CASE 2*a*, BATCH FRACTIONATION WITH CONSTANT REFLUX RATIO —SMALL NUMBER OF PLATES.

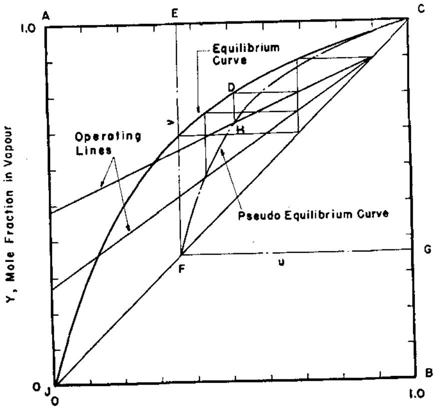

FIG. 4. CASE 2*b*. BATCH FRACTION PRODUCING CONSTANT COMPOSITION OF DISTILLATE — SMALL NUMBER OF PLATES.

$$y_{n-h} = r^h \left(\frac{\alpha}{\alpha + 1}\right) - b_1 \left(r^h + r^{h-1} + \right.$$

$$r^{h-s} + \ldots + r) + b_2 \left(r^{h-1} + \right.$$

$$\left. r^{h-2} + \ldots + 1\right) \quad (16)$$

If n is the number of equilibrium stages including the pot and if h is the number of theoretical plates in the column, then y_{n-h} is equal to y_1, the composition of the vapor from the first plate.

Summing the geometric series:

$$y_1 = \frac{r^h \left(\frac{\alpha}{\alpha + 1}\right) + b_2 \left(\frac{1 - r^h}{1 - r}\right)}{1 + \left(\frac{r}{R + 1}\right) \left(\frac{1 - r^h}{1 - r}\right)} \quad (17)$$

This gives one of the y values on the pseudoequilibrium curve *BHD,* the proposed curve relating the pot composition to the overhead composition for constant reflux ratio distillation for the given conditions. It is called a pseudoequilibrium curve because the constant relative volatility α' associated with it is to be used in the simple Rayleigh batch fractionation equation. The ordinates on the curve are denoted as y' to associate them with α'.

Again since the abscissa is still 0.5 for point *H,* the pseudorelative volatility α' is obtained from the ordinate.

$$\frac{\alpha'}{\alpha' + 1} = \frac{r^h \left(\frac{\alpha}{\alpha + 1}\right) + b_2 \left(\frac{1 - r^h}{1 - r}\right)}{1 + \left(\frac{r}{R + 1}\right) \left(\frac{1 - r^h}{1 - r}\right)} \quad (18)$$

where

$$r = \frac{\frac{2}{\alpha + 1}}{\frac{R}{R + 1}} = \frac{2 \, (R + 1)}{R \, (\alpha + 1)} \quad (19)$$

The pseudorelative volatility α' is now used in the same manner as true relative volatility in simple distillation. Mathematically, the pseudoequilibrium curve can be expressed in the equation

$$y' = \frac{\alpha' x}{1 + (\alpha' - 1) \, x} \quad (20)$$

By this development therefore the composition of distillate x_D corresponding to the liquid composition x in the pot at the same time is equal to the pseudovapor composition y' which is in equilibrium with the same liquid composition x. The closeness with which a curve so drawn follows the actual curve relating these compositions is indicated in the example shown in Figure 4. The dashed line *OJKHMD* was drawn here to relate actual pot compositions to overhead compositions for three theoretical plates. The curve *OEGFD* corresponds to an α' value based on Equation (18). Actually, at high values of x, y' will be found to be lower than x_D, as can be seen from Figures 3 and 5 and at lower x values y' will be greater than x_D. Nevertheless, for most applications the fit is sufficiently close for the results obtained to be useful. Equation (20) yields the approximation

$$x_D = \frac{\alpha' x}{1 + (\alpha' - 1)\,x} \qquad (21)$$

Substituting Equation (21) in the basic Rayleigh equation [Equation (4)] yields the relationship between the initial and final amounts of liquid in the pot:

$$\frac{W_i}{W} = \left[\frac{\dfrac{(1-x_i)^{\alpha'}}{x_i}}{\dfrac{(1-x)^{\alpha'}}{x}}\right]^{-\dfrac{1}{\alpha'-1}} \qquad (22)$$

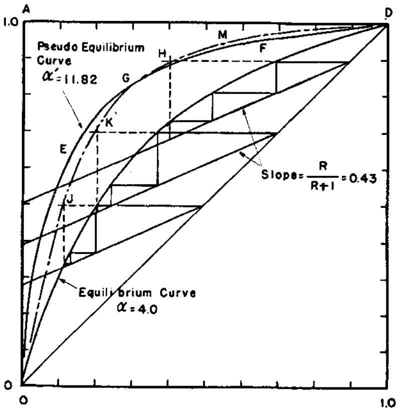

FIG. 5. SAMPLE CALCULATION OF CASE 2*a*.

And therefore the time required to reduce the liquid composition in pot from x_i to x is

$$\theta = (R+1)\,\frac{W_i}{V}\left\{1 - \left[\frac{\dfrac{(1-x_i)^{\alpha'}}{x_i}}{\dfrac{(1-x)^{\alpha'}}{x}}\right]^{\dfrac{1}{\alpha'-1}}\right\} \qquad (23)$$

Variable Reflux Ratio Producing Distillate of Constant Composition. Development of Equation (10) was made possible by the assumption that the operating line and equilibrium curve intersect at the abscissa corresponding to the pot composition. If the number of theoretical stages is relatively small, the composition of liquid in pot will correspond to a larger abscissa than this point of intersection. In the proposed method a pseudoequilibrium curve is set up which may be used in the same manner as for Equation (10) but which will reflect the small number of equilibrium stages. The pseudoequilibrium curve also includes the relative volatility of the system.

The method of introducing the pseudoequilibrium curve, illustrated in Figure 5, is to hold up to total reflux, and so the concentration of the pot liquid for the case of total reflux, a, is first obtained from the Fenske equation(*3*).

$$a = \frac{x_D}{\alpha^n (1 - x_D) + x_D} \qquad (24)$$

The pseudoequilibrium curve is now constructed based on the relations

$$u = (1 - a)x \qquad (25)$$

$$v = (1 - a)y \qquad (26)$$

The u-v coordinates now refer to a reduced diagram $EFGC$; the origin can be located as $x = a$ and $y = a$. The pseudoequilibrium curve is obtained by substituting u, v from above in Equation (1) to give

$$= \frac{\alpha u}{1 + \dfrac{(\alpha - 1)}{1 - a}\,u} = \frac{\alpha u}{1 + \beta\,(\alpha - 1)u} \qquad (27)$$

where

$$\beta = \frac{1}{1 - a} \qquad (28)$$

It should be emphasized that for this construction u-v and x-y coordinates adopt the same modulus. When it is desired to use x-y axes as a reference

$$x = u + a \qquad (29)$$

$$y = v + a \qquad (30)$$

Substituting these values in Equation (27) yields the correct form of the pseudoequilibrium curve referred to in the diagram $AOBC$ (x-y coordinates):

$$y = \frac{\alpha(x - a)}{1 + \beta\,(\alpha - 1)\,(x - a)} + a \qquad (31)$$

If one eliminates y between Equations (31) and (2) and solves for $(R + 1)$,

$$R + 1 = \frac{(x_D - x)\,[1 + \beta(\alpha - 1)X]}{(\alpha - 1)\,X\,(1 - \beta X)} \qquad (32)$$

where $X = x - a$

Equation (32) is the mathematical expression relating the reflux ratio, R, with the composition of pot liquid, x, for the case of a small number of theoretical stages and of distillate of constant composition. As

$$1 - \frac{L}{V} = \frac{1}{R + 1} \qquad (33)$$

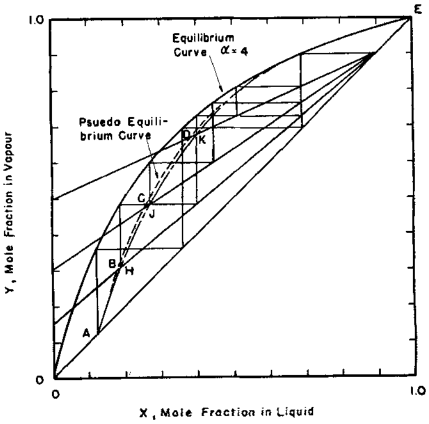

FIG. 6. SAMPLE CALCULATION OF CASE 2*b*.

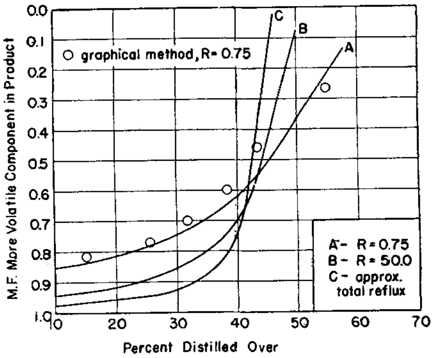

FIG. 7. SHARPNESS OF SEPARATION.

the proper substitutions can be made into Bogart's equation [Equation (8)] to yield finally

$$\theta = \frac{W_i\,(x_D - x_i)}{V\,(\alpha - 1)}\left[\frac{1}{m}\ln\frac{X_i}{X} + \frac{\alpha\beta}{m\beta - 1}\ln\frac{1 - \beta X}{1 - \beta X_i} + \frac{1 + m\beta\,(\alpha - 1)}{m\,(m\beta - 1)}\ln\frac{m - X_i}{m - X}\right] \qquad (34)$$

where

$X = x_i - a$
$X = x - a$
$m = x_D - a$

SHARPNESS OF FRACTIONATION FOR CONSTANT REFLUX RATIO AND A SMALL NUMBER OF PLATES

A sharpness of fractionation curve is a plot of the average dis-

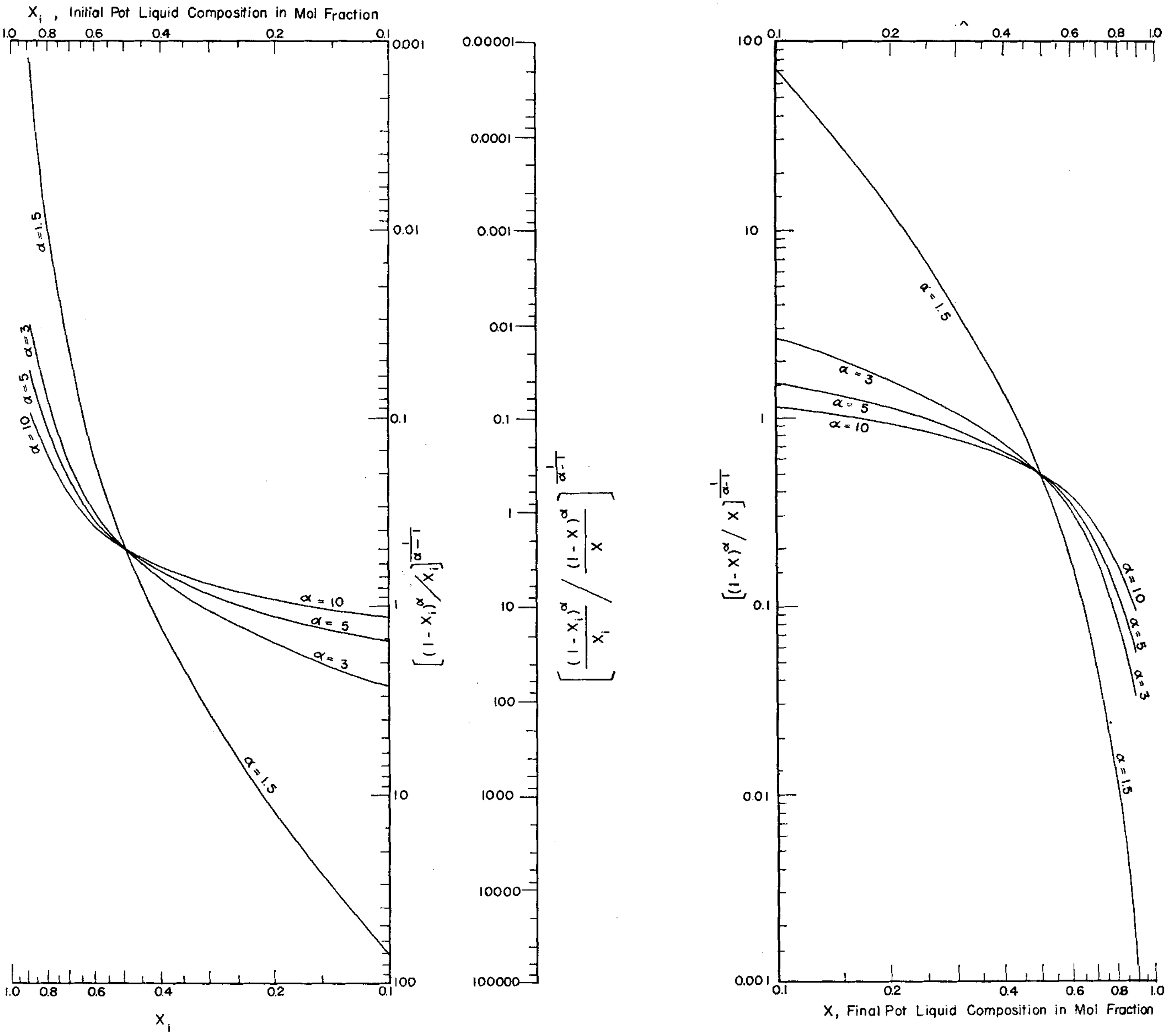

FIG. 8. NOMOGRAM FOR $\left[\frac{(1-x_i)^\alpha}{x_i} \Big/ \frac{(1-x)^\alpha}{x}\right]^{\frac{1}{\alpha-1}}$

tillate composition against the percentage of moles distilled. Rose and Welshans(6) have presented analytical methods for calculating sharpness curves for the case of constant relative volatility, any given number of stages, no holdup, and essentially total reflux.

Equation (22) will permit sharpness curves to be drawn for any reflux ratio, thus extending the work of Rose and Welshans. The pseudorelative volatility α' is calculated from Equation (18) as before. Figure 7 shows a series of curves corresponding to increasing reflux ratio to illustrate the calculation. Curve *A* is for a reflux ratio of 3 corresponding to the example of Figure 5; the circle points were calculated graphically for this example and show excellent agreement with the analytical results.

The calculations for curve *A* are shown as an appendix.

NOMOGRAMS

The final equations may be solved by combinations of nomograms of the usual type; however, there is little time advantage in using these, and for greater accuracy the use of the equations with a calculating machine is recommended.

Figure 8 is a nomograph for calculating

$$\left[\frac{\dfrac{(1-x_i)^\alpha}{x_i}}{\dfrac{(1-x)^\alpha}{x}}\right]^{\frac{1}{\alpha-1}}$$

which appears in Equations (6) and (23).

Figure 9 is a nomogram for calculating a based on Equation (24) and $\beta = \frac{1}{1-a}$. These values are required for the calculations utilizing Equation (34).

SAMPLE CALCULATIONS

As an illustration, the results of sample calculations are shown in Tables 1 and 2 and are compared with those obtained by graphical integration.

SUMMARY

The equations for approximate calculation to determine the time required to reduce the composition of liquid in the pot from x_i to x are summarized as follows:

I. Batch Operation Involving a Large Number of Theoretical Plates

a. Constant reflux ratio

$$\theta = (R+1)\frac{W_i}{V}\left\{1 - \left[\frac{\dfrac{(1-x_i)^{\alpha}}{x_i}}{\dfrac{(1-x)^{\alpha}}{x}}\right]^{\frac{1}{\alpha-1}\frac{1}{R+1}}\right\} \qquad (6)$$

b. Variable Reflux Ratio, Producing Distillate of Constant Composition

$$\theta = \frac{W_i\,(x_D - x_i)}{V(\alpha-1)x_D\,(1-x_D)}\left\{(1-x_D)\ln\frac{x_i}{x} + [1+(\alpha-1)x_D]\ln\frac{x_D - x}{x_D - x_i} + \alpha x_D \ln\frac{1-x_i}{1-x}\right\} \qquad (10)$$

II. Batch Operation Involving a Small Number of Theoretical Plates

a. Constant Reflux Ratio

$$\theta = (R+1)\frac{W_i}{V}\left\{1 - \left[\frac{\dfrac{(1-x_i)^{\alpha'}}{x_i}}{\dfrac{(1-x)^{\alpha'}}{x}}\right]^{\frac{1}{\alpha'-1}}\right\} \qquad (23)$$

where

$$\frac{\alpha'}{\alpha'+1} = \frac{r^h\left(\dfrac{\alpha}{\alpha+1}\right) + b_2\left(\dfrac{1-r^h}{1-r}\right)}{1 + \left(\dfrac{r}{R+1}\right)\left(\dfrac{1-r^h}{1-r}\right)}$$

$$r = \frac{2\,(R+1)}{R\,(\alpha+1)}, \text{ and } b_2 = \frac{\alpha-1}{\alpha+1}$$

b. Variable Reflux Ratio, Producing Distillate of Constant Composition

$$\theta = \frac{W_i\,(x_D - x_i)}{V\,(\alpha-1)}\left[\frac{1}{m}\ln\frac{X_i}{X} + \frac{\alpha\beta}{m\,\beta-1}\ln\frac{1-\beta X}{1-\beta X_i} + \frac{1+m\beta\,(\alpha-1)}{m\,(m\beta-1)}\ln\frac{m-X_i}{m-X}\right] \qquad (34)$$

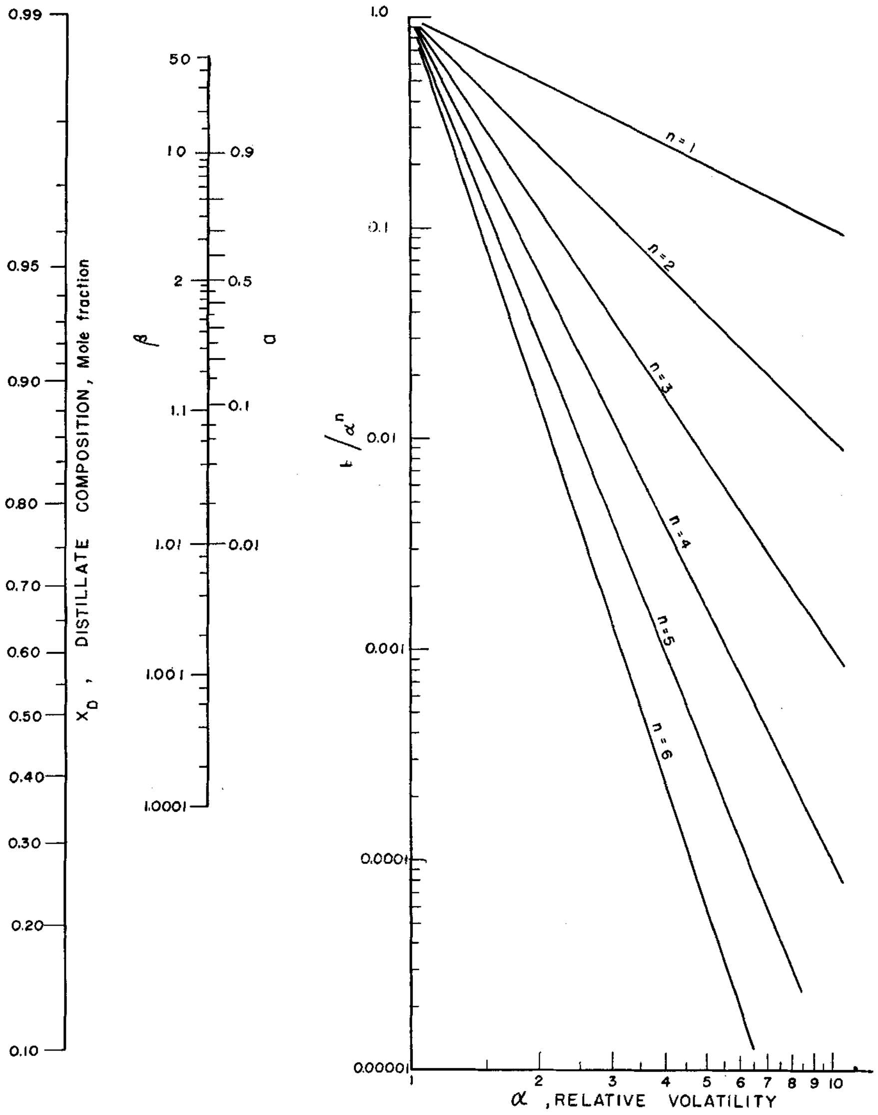

FIG. 9. NOMOGRAM FOR CONSTANTS α AND β.

where

$$X_i = x_i - a \qquad X = x - a$$

$$m = x_D - a \qquad \beta = \frac{1}{1-a}$$

and

$$a = \frac{x_D}{\alpha^n\,(1-x_D) + x_D}$$

TABLE 1.—BATCH OPERATIONS INVOLVING A LARGE NUMBER OF PLATES

Operating conditions and calculating results		Constant reflux ratio	Constant composition of distillate
Relative volatility	α	1.5	1.5
Initial amount of liquid in pot	W_i	100 moles	100 moles
Final composition of liquid in pot	x	0.05	0.05
Initial composition of liquid in pot	x_i	0.50	0.50
Rate of vaporization		50 moles/hr.	50 moles/hr.
Constant reflux ratio	R	3	
Initial reflux ratio	R_i	...	3
Constant composition of distillate	x_D	...	0.90
Composition of initial distillate	x_{D_i}	0.90	
Amount of liquid left in pot calculated by graphical integration	W	22.2 moles	
Amount of liquid left in pot calculated by proposed method [Equation (5)]	W	22.9 moles	
Time, calculated by graphical integration	θ	6.23 hr.	7.36 hr.
Time, calculated by proposed method		6.10 hr.	7.11 hr.

These equations involve novel pseudoequilibrium curves which may be useful in other applications, as illustrated by the example of sharpness of fractionation. It should be emphasized that these equations are approximate expressions only; however, they yield results which should aid in scheduling pilot-plant and industrial batch distillations and in evaluating the effect of the major factors—number of plates, relative volatility, vapor rates, and compositions on the times required for these distillations.

Some engineering discretion is required in the selection of equations. In general a small number of theoretical plates would be six or fewer and a large number ten or more. In border cases both equations should be applied for any given distillation.

NOTATION

W_i = Initial amount of liquid in pot, moles

W = Amount of liquid in pot, moles

x_i = Mole fraction of more volatile component of the initial liquid mixture in pot

x = Mole fraction of more volatile component of the liquid mixture in pot

α = Relative volatility

θ = Time required to reduce the initial liquid composition in pot, x_i, to the final composition, x, hr.

n = Number of theoretical stages

h = Number of theoretical plates in a distillation column

y = Vapor composition in mole fraction which is in equilibrium with liquid mixture of composition x

y' = Ordinate value on pseudo-equilibrium curve

R = Reflux ratio, L/D

R_i = Initial reflux ratio for the case of constant composition of distillate

V = Rate of vaporization, moles/hr.

L = Amount of reflux, moles/hr.

x_D = Mole fraction of more volatile component in the distillate

x_{D_i} = Mole fraction of more volatile component in the initial distillate for the case of constant reflux ratio

α' = Pseudorelative volatility determined by Equation (18)

a = Mole fraction of liquid calculated by Equation (24)

$\beta = 1/(1\text{-}a)$

$r = 2(R+1)/R(\alpha+1)$

$m_1 = R/(R+1)$

$m_2 = 2/(\alpha+1)$

$b_1 = x_D/(R+1)$

$b_2 = (\alpha-1)/(\alpha+1)$

$m = x_D - a$

$X_i = x_i - a$

$X = x - a$

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TABLE 2.—BATCH OPERATION INVOLVING A SMALL NUMBER OF PLATES

Operating conditions and calculation results		Constant reflux ratio	Constant composition of distillate
Relative volatility	α	4.0	4.0
Initial amount of liquid in pot	W_i	100 moles	100 moles
Initial composition of liquid in pot	x_i	0.40	0.40
Final composition of liquid in pot	x	0.10	0.18
Rate of vaporization	V	50 moles/hr.	50 moles/hr.
Number of theoretical stages	n	3	3
Number of theoretical plates in the column	h	2	2
Constant reflux ratio	R	0.75	
Initial reflux ratio	R_i	...	0.75
Constant composition of distillate	x_D	...	0.90
Initial composition of distillate	x_{D_i}	0.90	
r, calculated from Equation (19)	r	0.934	
Slope of pseudoline of Equation (12)	m_2	0.40	
Slope of operating line of Equation (13)	m_i	0.43	
b_2 of Equation (12)	b_2	0.60	
Pseudo relative volatility	α'	11.82	
a of Equation (24)	a	...	0.123
β calculated by Equation (28)	..	...	1.140
$m = x_D - a$	m	...	0.777
$X_i = x_i - a$	X_i	...	0.277
$X = x - a$	x	...	0.057
Time, calculated by graphical integration	θ	1.66 hr.	1.62 hr.
Time, calculated by proposed method	θ	1.50 hr.	1.48 hr.

(Presented at A.I.Ch.E. Washington meeting)

APPENDIX

Sharpness of Fractionation Curves by the Analytical Method

W = 100 moles
x_i = 0.40
n = 3
α = 4.0

	$R = 0.75$		$R = 50.0$		Total reflux*	
x	W	y	W	y	W	y
0.35	91.0	0.858	91.8	0.950	92.1	0.972
0.30	82.6	0.824	84.0	0.930	85.2	0.966
0.25	75.2	0.784	78.0	0.910	79.3	0.956
0.20	68.5	0.732	73.0	0.884	74.0	0.942
0.15	62.1	0.656	67.0	0.845	69.1	0.920
0.10	56.2	0.548	62.8	0.770	64.8	0.878
0.08	53.8	0.487	61.0	0.725	63.2	0.848
0.06	50.8	0.410	58.8	0.665	61.5	0.804
0.04	48.1	0.282	56.8	0.558	59.8	0.728
0.02	43.8	0.182	54.6	0.382	58.0	0.567

*According to Rose, A., and L. M. Welshans, *Ind. Eng. Chem.*, *32*, 668 (1940).

Graphical Construction

W = 100 moles
x_i = 0.40
n = 3
α = 4.0

x	W	y
0.35	92.0	0.858
0.30	83.2	0.820
0.25	74.5	0.768
0.20	68.4	0.700
0.15	61.7	0.600
0.10	56.2	0.460
0.05	45.2	0.265