Evaluation of the Heat Requirements in Batch Distillation Operations

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A rigorous method is presented for the evaluation of the heat requirements in binary batch fractionations which involve negligible column hold up. The method, in which the additional variables of the discontinuous process are taken into account, is a modification of the methods of Ponchon and Savarit for continuous operation. Two examples, one for a fractionation in which the composition of the product is constant and the other in which the reflux ratio is constant, are given as illustrations of the method.

The application of the method permits more accurate evaluation of reboiler and condenser heat loads and, in turn, better design.

The methods (*1, 6*) which are available for the solution of batch fractionation problems are often modifications of the McCabe-Thiele (*3*) solution for continuous-rectification problems. Consequently, the heat loads at the reboiler and condenser cannot be evaluated rigorously but can be only approximated. The degree of accuracy of the approximation depends upon the validity of the assumptions made in the McCabe-Thiele development: (1) molal latent heat independent of composition, (2) negligible heat of solution, and (3) negligible sensible heat effects. However, since the errors introduced by these individual assumptions may often tend to be compensating, better criteria for the applicability of the McCabe-Thiele method are that the saturated liquid and vapor lines on an enthalpy concentration are straight and, further, that the molal latent heat of vaporization is independent of composition. Either the chemical molecular weight or a fictitious molecular weight may be used as a basis for the determination of the molal latent heat.

Furthermore, when a modified McCabe-Thiele solution is applied to batch-fractionation problems, the condenser and reboiler loads become identical. For reasons cited above, it appears worth while to develop a method whereby the heat effects in batch distillation operations can be determined rigorously.

The methods of Ponchon (*4*) and Savarit (*5*) offer a rigorous means of solving two-component distillation problems in which the composition on a given plate is independent of time, i.e., steady state-operation. To apply this method to batch-fractionation problems, one must allow for the fact that the liquid and vapor compositions are functions of time as well as of plate number. Also one must take into account the fact that a batch fractionation may be carried out under conditions in which the product composition is constant and the reflux ratio varied or in which the reflux ratio is constant and the product composition allowed to change.

PROPOSED METHOD

The batch fractional-distillation system is shown diagrammatically in Figure 1. An over-all differential material balance is

$$dL = -dD \tag{1}$$

and an over-all differential-component material balance is

$$d(x_L L) = -x_D\,dD \tag{2}$$

Then, substituting Equation (1) into (2) gives

$$d(x_L L) = x_D\,dL \tag{3}$$

or

$$x_L\,dL + L\,dx_L = x_D\,dL \tag{4}$$

If Equation (4) is rearranged, an equation similar to the Rayleigh equation is obtained:

$$L^{-1}\,dL = (x_D - x_L)^{-1}\,dx_L \tag{5}$$

or

$$\ln(L/L_0) = \int_{x_{L_0}}^{x_L} (x_D - x_L)^{-1}\,dx_L \tag{6}$$

In a batch distillation in which the composition of the overhead production is held constant by variation of the reflux ratio, the preceding equation may be directly integrated. Substituting the integrated form of Equation (1) into this equation gives

$$D = L_0(x_{L_0} - x_L)/(x_D - x_L) \tag{7}$$

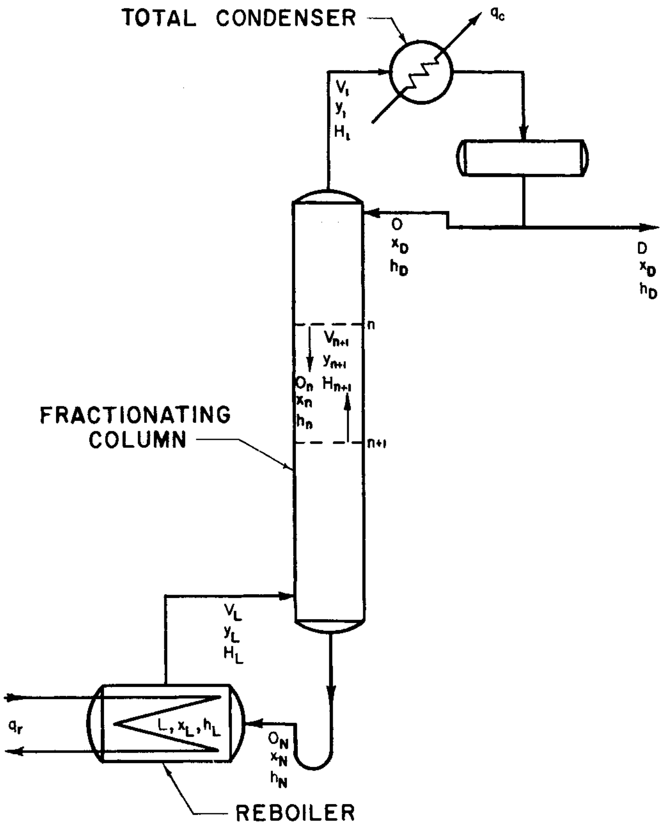

Fig. 1. Schematic diagram of a batch distillation system.

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This equation is simply a material balance. If x_D is replaced by $(x_D)_{avg}$ the equation is also valid for a batch distillation which is carried out by use of a constant reflux ratio.

To obtain equations relating the operating conditions in the column to the condenser load and product, heat and material balances are made around the n plate and the top of the column (Figure 1).

$$dD + d0_n = dV_{n+1} \tag{8}$$

$$x_D\, dD + x_n\, d0_n = y_{n+1}\, dV_{n+1} \tag{9}$$

and

$$d'q_c + h_D\, dD + h_n\, d0_n = H_{n+1}\, dV_{n+1} \tag{10}$$

Substituting Equation (8) into Equations (9) and (10) gives

$$d0_n/dD = (x_D - y_{n+1})/(y_{n+1} - x_n) \tag{11}$$

and

$$d0_n/dD = (d'q_c/dD + h_D - H_{n+1})/(H_{n+1} - h_n) \tag{12}$$

If

$$Q_c' = d'q_c/dD + h_D \tag{13}$$

Equation (12) may then be written

$$d0_n/dD = (Q_c' - H_{n+1})/(H_{n+1} - h_n) \tag{14}$$

The combination of Equations (11) and (14) gives

$$d0_n/dD = (x_D - y_{n+1})/(y_{n+1} - x_n) = (Q_c' - H_{n+1})/(H_{n+1} - h_n) \tag{15}$$

Equation (15) is equivalent to the equation developed by Ponchon (*4*) and Savarit (*5*) for the operating line in the rectifying section for the solution of problems involving continuous fractionation processes.

If Equation (15) is applied to the top of the column, the relationship between Q_c' and the reflux ratio is obtained:

$$\frac{d0}{dD} = \frac{Q_c' - H_1}{H_1 - h_D} \tag{16}$$

If the complete system is considered, an over-all heat balance may be written:

$$d'q_r = d'q_c + h_D\, dD + d(h_L L) \tag{17}$$

or

$$d'q_r = Q_c'\, dD + d(h_L L) \tag{18}$$

It should be noted that Equations (17) and (18) imply adiabatic operation of the column and neglect the temperature changes of the materials of construction. Equations (6), (13), (15), and (18) are sufficient to solve rigorously any binary batch distillation problem with negligible liquid holdup.

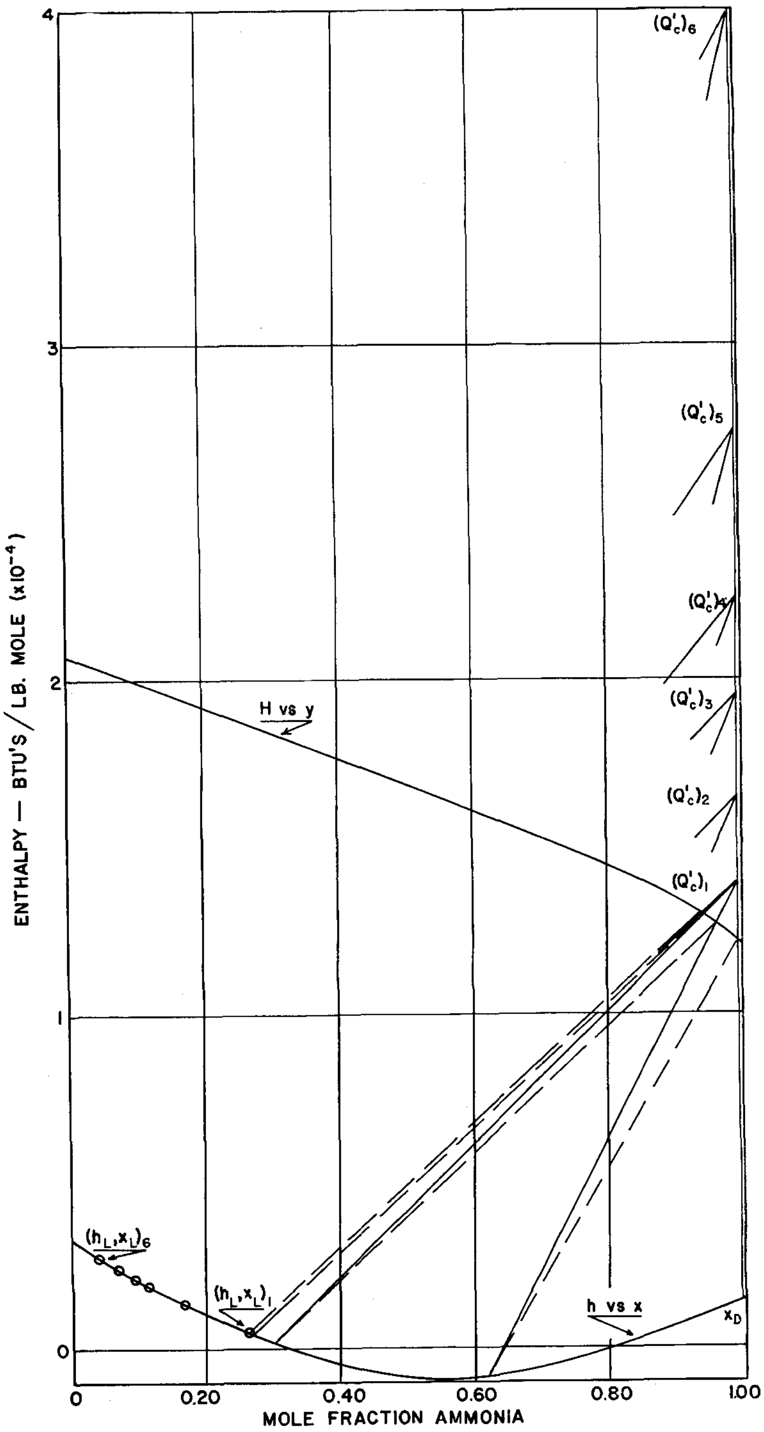

Fig. 2. Enthalpy-concentration diagram for the ammonia-water system showing the variation of Q_c' and x_L when x_D is held constant.

Equation (15) and an enthalpy-concentration diagram for the system under consideration provide a graphical method of determining the relationship between the still composition, the distillate composition, and the reflux ratio as shown by Ponchon and Savarit. Equations (13) and (18) provide the relationships necessary to solve rigorously for the heat requirements.

Equation (18) may be integrated to give

$$q_r = \int_0^D Q_c'\, dD + h_L L - h_{L_0} L_0 \tag{19}$$

Rearranging and integrating Equation (13) results in the following equation:

$$q_c = \int_0^D Q_c'\, dD - \int_0^D h_D\, dD \tag{20}$$

The integration of $Q_c'\, dD$ in Equations (19) and (20) must necessarily be carried out graphically, the relationship between Q_c' and D being found from Equations (1), (6), and (15).

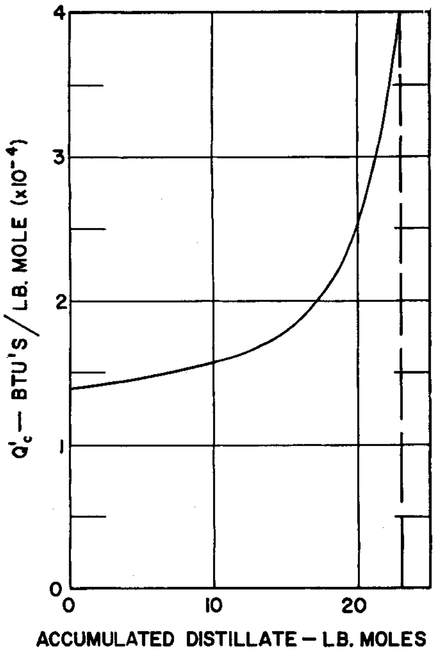

Fig. 3. Q_c' vs. D plot for the evaluation of $\int_0^D Q_c'\,dD$.

Equation (20) may be simplified when the method of operation is such that the overhead product composition is constant, as h_D is dependent only upon the product composition.

$$q_c = \int_0^D Q_c'\,dD - h_D D \qquad (21)$$

When the method of operation is such that the reflux ratio is constant, $h_D\,dD$ must be graphically integrated for a rigorous solution of Equation (20). However, for some systems the saturated liquid line on an enthalpy-concentration diagram is nearly a straight line. If the enthalpy of the product leaving the system when approximately half the product has been collected can be estimated, Equation (20) may be simplified to give

$$q_c = \int_0^D Q_c'\,dD - (h_D)_{avg} D \qquad (22)$$

Equation (22) should not result in any significant error if the saturated liquid line is nearly horizontal.

ILLUSTRATIONS

Two illustrations, one for the case of constant product composition and the other for the case of constant reflux ratio, are presented here to compare the results obtained by previously developed methods with the results obtained by the rigorous method presented here. The ammonia-water system was used in both illustrations and the data of Merkel and Baznjakowic (*2*) were utilized.

The first problem considered was

L_0 = 100 lb. moles
x_{L_0} = 0.258 NH_3 (mole fraction)
x_D = 0.995 NH_3 (mole fraction)
x_L(final) = 0.039 NH_3 (mole fraction)
Reflux ratio—variable
Number of theoretical plates = 4
Pressure = 14.7 lb./sq. in. abs.

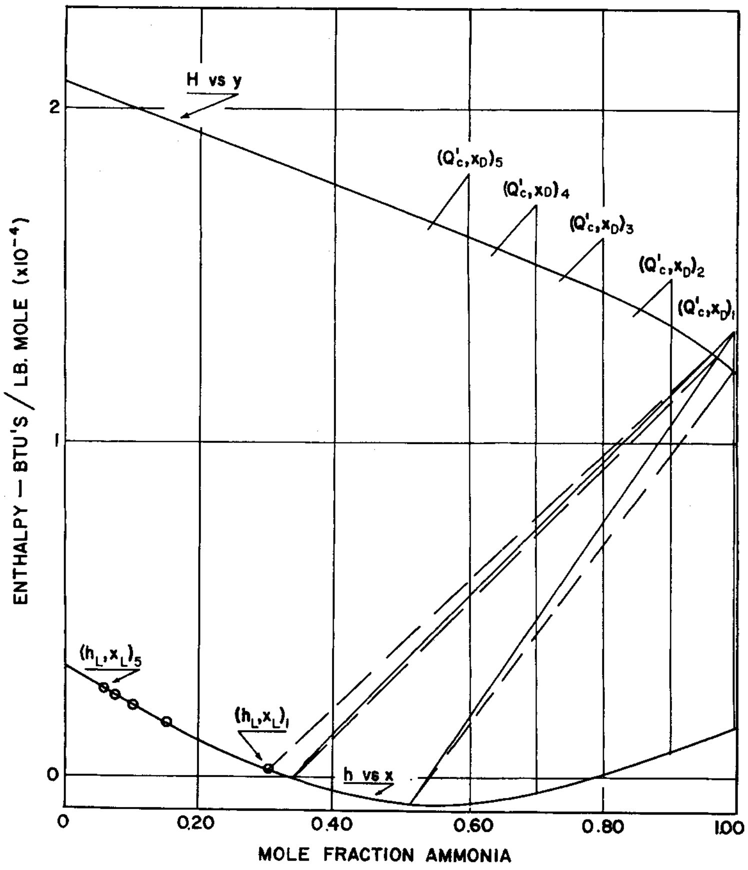

Fig. 4. Enthalpy-concentration diagram for the ammonia-water system showing the variation of Q_c' and x_L when the reflux ratio is constant.

With the information given above and Equation (7), the top product obtained is 22.91 moles.

If this problem is solved by the method of Bogart (*1*), a fictitious molecular weight for one of the components must be used if the necessary assumptions are to be approximately true. No one value for the fictitious molecular weight will satisfy the requirements; consequently, different results will be obtained depending upon the value selected. A fictitious molecular weight of 29.7 for ammonia was chosen for this illustration. This value was determined by making the molal latent heat of vaporization of ammonia equal to the molal latent heat of vaporization of water. The problem was then solved and it was determined that 20.16 fictitious moles of vapor entered the condenser. If the molal latent heat of condensation of water is used, the heat load at the condenser is

$$q_c = (20.16)(17{,}484)$$

$$= 352{,}000 \text{ B.t.u.}$$

The heat load at the reboiler is identical, owing to the assumptions made. In the solution of the problem the operating lines were considered straight, an assumption that is unrealistic for this system.

If this problem is solved by the proposed method, the procedure would be:

1. On an enthalpy-concentration diagram for the ammonia-water system, locate x_D at 0.995 mole fraction ammonia and assume a value for Q_c'. The reflux ratio is then fixed.
2. Step off four theoretical plates and thus determine x_L. (See Figure 2.)
3. Use Equation (6) to determine the amount of distillate obtained.
4. Repeat steps 1 to 3, using different values of Q_c'. This permits the determination of Q_c' as a function of the number of moles of distillate accumulated.
5. Plot Q_c' as a function of the accumulated distillate (Figure 3) and by graphical integration determine the value of $\int_0^D Q_c'\,dD$, the first term in the right-hand member of Equation (21).
6. Determine the condenser heat load by Equation (21).
7. Determine the reboiler heat load by Equation (19).

For the problem in question,

$$\int_0^{22.9} Q_c'\,dD = 426{,}000 \text{ B.t.u.}$$

and

$$q_c = 426{,}000 - (1{,}410)(22.91)$$

$$q_c = 394{,}000 \text{ B.t.u.}$$

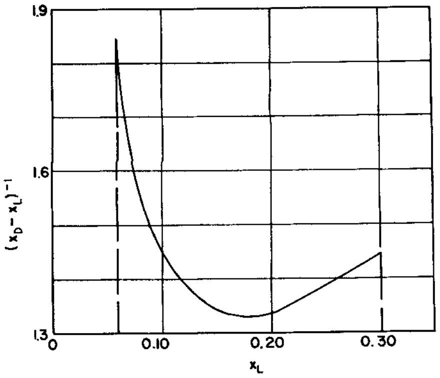

Fig. 5. $(x_D - x_L)^{-1}$ vs. x_L plot for the evaluation of $\int_{x_{L_0}}^{x_L} (x_D - x_L)^{-1}\, dx_L$.

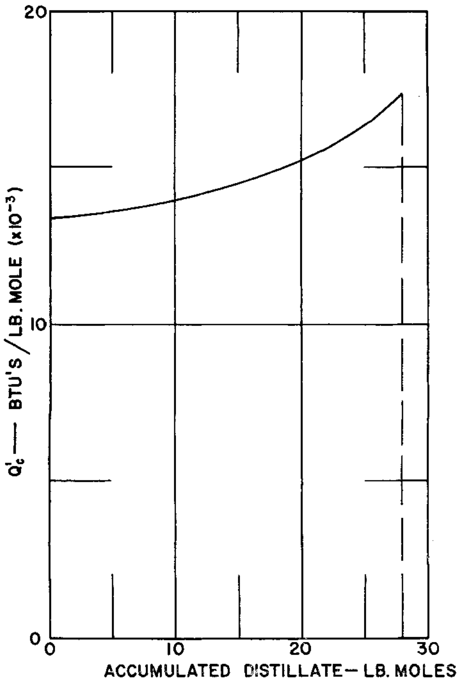

Fig. 6. Q_c' vs. D plot for the evaluation of $\int_0^D Q_c'\, dD$.

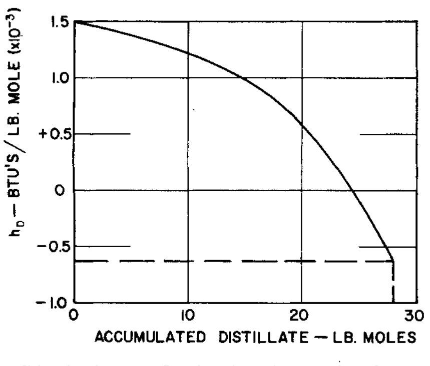

Fig. 7. h_D vs. D plot for the evaluation of $\int_0^D h_D\, dD$.

and

$$q_r = 426{,}000 + (77.09)(2{,}700) - (100)(-890)$$

$$q_r = 723{,}000 \text{ B.t.u.}$$

It will be noted that the reboiler heat loads, as determined by the two methods, are hardly comparable and that the condenser heat loads differ by 10.7%.

The second illustration is one in which the reflux ratio was held constant and the composition of the overhead product allowed to vary. The problem was

L_0 = 100 lb. moles
x_{L_0} = 0.302 NH_3 (mole fraction)
$(x_D)_{avg}$ = 0.90 NH_3 (mole fraction)
$0/V_1$ = 0.10
Number of theoretical plates = 3
Pressure = 14.7 lb./sq. in. abs.

If a fictitious molecular weight of 29.7 for ammonia is assumed and the problem solved by the method of Smoker and Rose (*6*), it is determined that 21.3 fictitious moles of vapor enter the condenser. If the molal latent heat of condensation of water is used, the heat load at the condenser is

$$q_c = (21.3)(17{,}485) = 372{,}000 \text{ B.t.u.}$$

The reboiler and condenser heat loads are identical in this method.

By the proposed method of solution, the following procedure is used:

1. On an enthalpy-concentration diagram for the ammonia-water system, assume a value of x_D (this fixes h_D) and locate Q_c'. Q_c' can be calculated, since the $0/V_1$ ratio is fixed. (See Figure 4.)
2. Step off three theoretical plates and determine x_L and h_L.
3. Use Equation (6) to determine the amount of distillate obtained. (See Figure 5.)
4. Repeat steps 1 to 3 and plot $(x_D)_{avg}$ vs. accumulated distillate. From this plot the amount of product of 0.90 NH_3 can be obtained. This particular step is basically the same procedure as used in the Smoker and Rose method.
5. Plot Q_c' as a function of the amount distilled (Figure 6) and determine the value of $\int_0^D Q_c'\, dD$.
6. Plot h_D as a function of the amount distilled (Figure 7) and determine the value of $\int_0^D h_D\, dD$.
7. Determine the reboiler heat load by Equation (19).
8. Determine the condenser heat load by Equation (20).

For the problem in question:

$$\int_0^{28.0} Q_c'\, dD = 405{,}000 \text{ B.t.u.}$$

$$\int_0^{28.0} h_D\, dD = 11{,}000 \text{ B.t.u.}$$

therefore,

$$q_r = 405{,}000 + (2{,}660)(72) - (195)(100)$$

$$q_r = 577{,}000 \text{ B.t.u.}$$

and

$$q_c = 405{,}000 - 11{,}000$$

$$q_c = 394{,}000 \text{ B.t.u.}$$

Although the heat loads at the condenser, as calculated by the two methods, differ by only 5.6%, the heat loads at the reboiler differ by 35.4%.

SUMMARY

A rigorous method for the determination of the heat requirements in batch fractionation processes has been presented. The method, which is a modification of the methods of Ponchon (*4*) and Savarit (*5*), can be used for the solution of batch-fractionation problems in which the reflux ratio is constant and the overhead product varies or in which the overhead product is constant and the reflux ratio varies.

The proposed method is illustrated and compared with methods which have been presented previously.

NOTATION

D = amount of product
H = enthalpy per unit quantity of vapor
L = amount of liquid in still
O = amount of liquid overflow
Q_c' = construction point representing conditions at top of column
V = amount of vapor flow
d = differential
d' = inexact differential
h = enthalpy per unit quantity of liquid
q_c = amount of heat removed at the condenser
q_r = amount of heat added at the reboiler
x = composition in the liquid phase
y = composition in the vapor phase

Subscripts

D = product
L = still
L_0 = initial still conditions
N = bottom plate in column
n = nth plate in column
$n + 1$ = $(n + 1)$ plate in column
1 = top plate

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