

EXTENDED SMOKER'S EQUATION FOR CALCULATING NUMBER OF STAGES IN DISTILLATION

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In 1938, Smoker proposed an analytical closed form formula to calculate the number of stages in a binary distillation column. The equation assumes constant relative volatility and constant molar overflow. For many mixtures, it is practical to assume constant relative volatility. However, the latent heat of vaporization of the different components are generally not equal and hence, the analytical formula fails to predict the number of equilibrium stages with reasonable accuracy. Due to this non-uniform latent heat requirement, the operating lines in McCabe-Thiele diagram are no longer straight but curved. In this paper, a closed form formula is derived without assuming the constant molar overflow. Proposed extended formula predicts the number of equilibrium stages in a binary distillation with constant relative volatility and unequal latent heat requirement.

INTRODUCTION

In distillation, the McCabe-Thiele (1925) or any other graphical method becomes inconvenient if a large number of stages are required to effect the desired separation. Smoker (1938) proposed an analytical closed form formula to calculate the number of stages in a binary distillation column along with the assumptions of constant relative volatility and constant molar overflow. The Smoker (1938) equation is convenient to use to calculate number of equilibrium stages and can be applied for computer based optimization procedure. However, without the assumption of constant molar overflow, the operating line on the McCabe-Thiele (1925) diagram becomes curved and the analysis becomes cumbersome (Smith, 1963). In such cases, it is better to use the graphical methods of Ponchon (1921) and Savarit (1922), which includes the enthalpy balances in the graphical construction. Jafarey et al. (1979) developed a simplified approximate solution of Smoker (1938) equation.

For many mixtures, it is practical to assume constant relative volatility. However, the latent heat of vaporization of the different components are generally not equal and hence, the Smoker (1938) equation fails to predict the number of equilibrium stages with reasonable accuracy. In this paper, an analytical equation is presented to compute the number of theoretical stages in binary distillation when the enthalpy-composition lines are straight but not parallel. By assuming non-parallel enthalpy-composition lines, the constant molar overflow assumption in the original Smoker (1938) equation is relaxed. Proposed extended formula predicts the number of equilibrium stages in a binary distillation with constant relative volatility and unequal latent heat requirement.

EQUILIBRIUM AND OPERATING LINES

Equilibrium curve for binary distillation with constant relative volatility of α can be represented analytically as

$$y = \frac{\alpha x}{1 + (\alpha - 1)x} \quad \text{or} \quad x = \frac{y}{\alpha - (\alpha - 1)y} \quad (1)$$

Overall mass, species, and overall energy balances in the rectifying section (Figure 1a) may be expressed as

$$V = L + D \quad (2)$$

$$Vy = Lx + Dx_d \quad (3)$$

$$Vh_v = Lh_l + Dh_d + Q_c \quad (4)$$

Note that the overall energy balance equation (4) is expressed in terms of the condenser duty (Q_c). This will enable us to compute the number of stages from a single formula for different types of condenser (total or partial).

Solving energy (4) and overall mass (2) balances

$$L = \frac{Q_c}{h_v - h_l} + D \frac{h_d - h_v}{h_v - h_l} \quad (5)$$

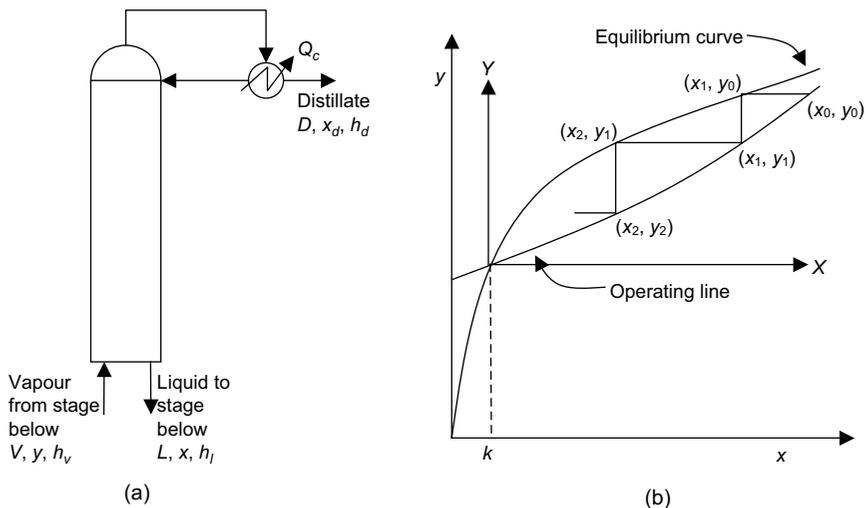


Figure 1. (a) Rectifying section of a distillation column. (b) Intersection of equilibrium and operating lines, associated coordinate transformation and stage calculation

$$V = \frac{Q_c}{h_v - h_l} + D \frac{h_d - h_l}{h_v - h_l} \quad (6)$$

In this paper, we assume vapour and liquid phase specific enthalpies are linear function composition.

$$h_l = h_l^0 + ax \quad (7)$$

$$h_v = h_v^0 + by \quad (8)$$

Combining equations (7) and (8) with equations (5) and (6), liquid and vapour flows can be calculated as

$$L = \frac{Q_c}{(h_v^0 - h_l^0) + (by - ax)} + D \frac{(h_d - h_v^0 - by)}{(h_v^0 - h_l^0) + (by - ax)} \quad (9)$$

$$V = \frac{Q_c}{(h_v^0 - h_l^0) + (by - ax)} + D \frac{(h_d - h_l^0 - ax)}{(h_v^0 - h_l^0) + (by - ax)} \quad (10)$$

Operating line represents the species balance equation (3) in a distillation. Liquid and vapour flow rate expressed in equations (9) and (10) may be combined with species balance equation (3), to obtain the operating line for binary distillation linear enthalpy-composition relationship.

$$y = (L/V)x + (D/V)x_d = \frac{Q_c + D(h_d - h_v^0 - by)}{Q_c + D(h_d - h_l^0 - ax)}x + D \frac{(h_v^0 - h_l^0) + (by - ax)}{Q_c + D(h_d - h_l^0 - ax)}x_d \quad (11)$$

This may be further simplified to

$$y = \frac{c_3 + x}{c_1 - c_2x} \quad (12)$$

where

$$c_1 = 1 + \left(\frac{D}{Q_c + D(h_d - h_v^0 - ax_d)} \right) (h_v^0 - h_l^0) + \left(\frac{D}{Q_c + D(h_d - h_v^0 - ax_d)} \right) (a - b)x_d \quad (13)$$

$$c_2 = \left(\frac{D}{Q_c + D(h_d - h_v^0 - ax_d)} \right) (a - b) \quad (14)$$

$$c_3 = \left(\frac{D}{Q_c + D(h_d - h_v^0 - ax_d)} \right) (h_v^0 - h_l^0)x_d \quad (15)$$

It may be noted that the operating line (i.e., equation (11) or (12)) is no longer straight. The assumption of parallel enthalpy-composition lines (i.e., constant molar overflow) implies $c_2 = 0$ as $a = b$ and equation (12) simplified to a straight line.

Similar to equation (12), operating line for the stripping section may be derived. It will have essentially the same form as in equation (12) where constants should be changed as follows.

$$c_1 = 1 - \left(\frac{B}{Q_r - B(h_b - h_v^0 - ax_b)} \right) (h_v^0 - h_l^0) - \left(\frac{B}{Q_r - B(h_b - h_v^0 - ax_b)} \right) (a - b)x_b \quad (16)$$

$$c_2 = - \left(\frac{B}{Q_r - B(h_b - h_v^0 - ax_b)} \right) (a - b) \quad (17)$$

$$c_3 = \left(\frac{-B}{Q_r - B(h_b - h_v^0 - ax_b)} \right) (h_v^0 - h_l^0)x_b \quad (18)$$

TRANSFORMATION

Intersection of the equilibrium line with the operating curve (within any given section of the column) may be obtained (Figure 1b) by solving equations (1) and (12).

$$x^2(\alpha - 1 + \alpha c_2) + x[1 + c_3(\alpha - 1) - \alpha c_1] + c_3 = 0 \quad (19)$$

The assumptions of constant relative volatility and single feed column imply that the intersection of the operating line and the equilibrium curve (i.e., root of equation (19)) will lie between 0 and 1. Let, the solution of the above equation be $x = k$, such that $0 \leq k < 1$ (Figure 1b) and corresponds to this solution, $y = (c_3 + k)/(c_1 - c_2 k)$.

It is now convenient to transform the equilibrium and operating lines by shifting the origin of the x-y axes to the intersection point. Similar transformation was originally proposed by Smoker (1938). Transformation equations between the two sets of coordinate axes are expressed as follows (Figure 1b).

$$X = x - k \quad (20)$$

$$Y = y - \frac{c_3 + k}{c_1 - c_2 k} \quad (21)$$

Transformed equilibrium and operating lines may be expressed as

$$X = \frac{(1 + \alpha k - k)^2 Y}{\alpha - (1 + \alpha k - k)(\alpha - 1)Y} \quad (22)$$

$$Y = \frac{(c_2 c_3 + c_1) X}{(c_1 - c_2 k)(c_1 - c_2 k - c_2 X)} \quad (23)$$

STAGE CALCULATION

Let us now start at some point (x_0, y_0) on the operating line in Figure 1b (say the overhead product purity). By alternate use of equations (22) and (23), coordinate of the next stage can be calculated as below.

$$Y_0 = \frac{(c_2c_3 + c_1)X_0}{(c_1 - c_2k)(c_1 - c_2k - c_2X_0)} \quad (24)$$

$$\begin{aligned} X_1 &= \frac{(1 + \alpha k - k)^2 Y_0}{\alpha - (1 + \alpha k - k)(\alpha - 1)Y_0} \\ &= \frac{(1 + \alpha k - k)^2 \frac{(c_2c_3 + c_1)X_0}{(c_1 - c_2k)(c_1 - c_2k - c_2X_0)}}{\alpha - (1 + \alpha k - k)(\alpha - 1) \frac{(c_2c_3 + c_1)X_0}{(c_1 - c_2k)(c_1 - c_2k - c_2X_0)}} \\ &= \frac{M_1 X_0}{\alpha - (M_2 \alpha - M_3) X_0} \end{aligned} \quad (25)$$

where

$$M_1 = \frac{(1 + \alpha k - k)^2 (c_2c_3 + c_1)}{(c_1 - c_2k)^2} \quad (25)$$

$$M_2 = \frac{(c_1 - c_2k)c_2 + (1 + \alpha k - k)(c_2c_3 + c_1)}{(c_1 - c_2k)^2} \quad (26)$$

$$M_3 = \frac{(1 + \alpha k - k)(c_2c_3 + c_1)}{(c_1 - c_2k)^2} \quad (27)$$

Repeating the above procedure of alternate use of material balance and equilibrium relation, until stage n is reached, gives the relation between x_0 and x_n as

$$X_n = \frac{M_1^n X_0}{\alpha^n - \left(\frac{M_2 \alpha - M_3}{\alpha - M_1} \right) (\alpha^n - M_1^n) X_0} \quad (28)$$

The above relation may easily be proved by induction. Rearranging equation (28) we get,

$$\left(\frac{\alpha}{M_1} \right)^n = \frac{X_0 \left[1 - \left(\frac{M_2 \alpha - M_3}{\alpha - M_1} \right) X_n \right]}{X_n \left[1 - \left(\frac{M_2 \alpha - M_3}{\alpha - M_1} \right) X_0 \right]} \quad (29)$$

Taking logarithm on both sides, number of stages may be calculated analytically as

$$n = \frac{\ln \left(\frac{X_0}{\left[1 - \left(\frac{M_2 \alpha - M_3}{\alpha - M_1} \right) X_0 \right]} \middle/ \frac{X_n}{\left[1 - \left(\frac{M_2 \alpha - M_3}{\alpha - M_1} \right) X_n \right]} \right)}{\ln \left(\frac{\alpha}{M_1} \right)} \quad (30)$$

Equation (30) must be applied separately to the rectifying and stripping sections to calculate the theoretical stage requirement in both sections of the column. While applying equation (30) separately in rectifying and stripping section, care should be taken in terms of satisfying mass, material and energy balances over the entire column.

SPECIAL CASES

For systems where the enthalpy-composition lines are parallel to each other (i.e., constant molar overflow), $a = b = 0$. It implies that $c_1 = (R + 1)/R$, $c_2 = 0$, and $c_3 = x_d/R$. Hence, $M_1 = R(1 + \alpha k - k)^2/(R + 1)$ and $M_2 = M_3 = (1 + \alpha k - k)R/(R + 1)$. Substituting these values in the final equation (30), the Smoker (1938) equation is obtained.

Whenever the distillation column operates with total reflux, condenser load may be mathematically assumed to be infinity ($Q_c \rightarrow \infty$). It implies that $c_1 = 1$, and $c_2 = c_3 = 0$ and hence, $M_1 = M_2 = M_3 = 1$. Substituting these values in the final equation (30), Fenske (1932) equation for calculating minimum number of stages at total reflux may be obtained.

$$n = \frac{\ln \left(\frac{X_0}{[1 - X_0]} \middle/ \frac{X_n}{[1 - X_n]} \right)}{\ln(\alpha)} = \frac{\ln \left(\frac{x_0}{[1 - x_0]} \middle/ \frac{x_n}{[1 - x_n]} \right)}{\ln(\alpha)} \quad (31)$$

It may be noted that at total reflux operating line becomes a straight line ($y = x$ line) and intersects the equilibrium curve at origin and at unity (i.e., $k = 0, 1$). Therefore, there is no requirement of shifting the coordinate axes.

Let the intersection of the q -line of the feed with the equilibrium curve be denoted as (x^*, y^*) . At minimum reflux, the intersection of the operating line with the equilibrium curve (equation (19)) must be (x^*, y^*) . This is ensured by the constant relative volatility assumption. For saturated liquid feed, solution of equation (19) results in minimum reflux.

$$R_{\min} + 1 = \frac{(x_d - x^*) \left[h_v^0 - h_l^0 + y^*(b - a) \right]}{(y^* - x^*) \left[h_v^0 - h_l^0 + x_d(b - a) \right]} \quad (32)$$

EXAMPLE

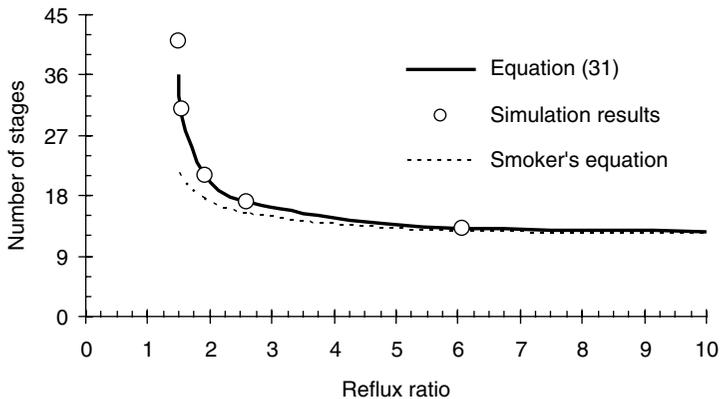
To illustrate the applicability of the analytical formula, a simple benzene-toluene example is considered. Feed and column data are given in Table 1. HYSIS (2003) is used a

Table 1. Data for benzene-toluene example

System	Benzene-Toluene	
Thermodynamic method	SRK	
Operating pressure	1 atm	
Feed data	Flow rate	100 kgmol/h
	Composition	50% benzene
	Pressure	1 atm
	Temperature	Due point
Specifications	Top	99% benzene
	Bottom	99% toluene

simulation tool. In detailed simulation, thermodynamic properties, including vapour-liquid equilibrium, have been calculated based on Soave-Redlich-Kwong (SRK) equation of state. From a converged simulation of a 20 stage column (excluding total condenser and partial reboiler), it is observed that the relative volatilities at the top and at the bottom of the column are 2.44 and 2.076, respectively. It shows that for a simple system like benzene-toluene, there is a 7.2% variation in relative volatility. Based on the geometric mean, the relative volatility of the benzene-toluene system is estimated to be 2.356 (Douglas, 1988). Enthalpy composition profiles, obtained from the converged simulation, show a linear relationship. Constants in equations (7) and (8) are estimated to be (in kJ/kmol) $h_1^0 = 26219$, $h_2^0 = 60017$, $a = 30534.55$, and $b = 27849$, with unity coefficient of determination.

Based on the above estimated parameters, the minimum number of stages is calculated to be 7. Since, at total reflux the operating line coincides with the $x = y$ line,

**Figure 2.** Number of theoretical stages in benzene-toluene system estimated using different methods

predicted minimum number of stages (31) are identical in both Smokers (1938) equation and equation (30). Based on equation (32), the minimum reflux is calculated to be 1.485. The minimum reflux predicted from the Smoker's equation is 1.425. Operating reflux of 100 stage column, as obtained from a converged simulation, is 1.489. Detail comparison between proposed analytical formula (30) and Smoker (1938) equation against simulation results (based on SRK equation of state) are shown in Figure 2. It may be seen that the proposed formula predicts number of stages more accurately than Smoker equation, especially, at lower reflux.

CONCLUSION

Most popular method for fast estimating number of stages in a distillation column is the short cut design method based on Fenske-Underwood-Gilliland procedure. In this procedure, minimum number of stages is estimated by Fenske (1932) equation, minimum reflux is estimated using Underwood (1946) equation, and the number of stages are estimated using graphical chart (Robinson and Gilliland, 1950) or simple equation (Eduljee, 1975) of Gilliland correlation. This procedure can be applied for multicomponent system. For binary system Smoker (1938) equation can be used to estimate number of theoretical stages.

The extended Smoker (1938) equation, presented in this paper, may be directly applied to predict the actual number of stages. Through a numerical simulation it has been observed that the proposed equation predicts number of theoretical stages with reasonable accuracy, especially at lower reflux.

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