J. King Saud Univ., Vol. 21, *Eng. Sci.* (1), pp. 1-5, Riyadh (2009/1430H.)

A Shortcut Method for Binary Distillation Column Design

Moustafa A. Soliman
Chemical Engineering Department, King Saud University
P.O. Box 800, Riyadh 11421, Saudi Arabia
mostf34@hotmail.com

(Received 11/4/2007; accepted for publication 10/7/2007)

Keywords: Binary Distillation, Shortcut, Design, Number of stages, Smoker equation.

Abstract. Based on Smoker (1938) analytical solution for binary distillation with constant relative volatility, Jafarey *et al.* (1979) derived a simple approximate design equation for the number of theoretical stages. This equation is modified to improve its predictions. This modified equation is particularly useful in computer process control applications because it gives an expression for the separation factor which is independent of the output parameters.

Introduction

There are many expressions for relating the number of stages in distillation to the reflux ratio, and relative volatility. Gilliland (1940) expressed this relation in a graphical form. The graphical plot was then correlated in analytical form by many investigators. One of these equations derived by Molokanov *et al.* (1972) takes the form:

$$\frac{N-N_{\min}}{N+1}=1-\exp\left[\left(\frac{1+54.4X}{11+117.2X}\right)\left(\frac{X-1}{X^{0.5}}\right)\right] \qquad (1)$$

where

$$X=\frac{R-R_{\min}}{R+1}$$

N is the number of plates
$N_{\min}$ is the minimum number of plates
R is the reflux ratio
$R_{\min}$ is the minimum reflux ratio

Jafarey *et al.* (1979) obtained an expression for the number of plates in terms of the separation factor (S) given by:

$$S=\frac{x_d(1-x_b)}{(1-x_d)x_b}$$

where x_d, and x_b are the mole fractions of the light component at the top and bottom respectively.

This expression can be used to relate the separation factor to the number of stages, reflux ratio, and relative volatility. The separation factor is useful in obtaining analytical expressions for the steady states gain as indicated by Skogestad and Morari (1987). They also obtained an analytical expression for the separation factor which gives predictions similar to Jafarey's *et al.* expression.

Mathematical Development

If we assume that α (relative volatility) is constant and that the molar flows are constant (the McCabe Thiele assumption), then for the rectifying section, the operating line is:

$$y=mx+b \qquad (20$$

where m is the slope of the line and is given by:

$$m=R/(R+1) \qquad (3)$$

and b is the intercept given by:

$$b = x_d/(R+1) = x_d(1-m) \tag{4}$$

R is the reflux ratio

x_d is the distillate mole fraction

Smoker (1938) was able to obtain an analytical expression to calculate the number of plates in the rectifying section N_R by the equation,

$$N_R = \frac{\log\left\{\dfrac{\bar{x}_o\left[1-\left(\dfrac{mc_1(\alpha-1)\bar{x}_n}{\left(\alpha-mc_1^2\right)}\right)\right]}{\bar{x}_n\left[1-\left(\dfrac{mc_1(\alpha-1)\bar{x}_o}{\left(\alpha-mc_1^2\right)}\right)\right]}\right\}}{\log\left\{\dfrac{\alpha}{mc_1^2}\right\}} \tag{5}$$

where

$$c_i = 1+(\alpha-1)k_i \qquad ,i=1,2 \tag{6}$$

$$\bar{x}_o = x_o - k_1 \tag{7}$$

$$\bar{x}_n = x_n - k_1 \tag{8}$$

k_i 's are the root of the quadratic ($0 < k_1 < 1$)

$$m(\alpha-1)k^2 + [m + b(\alpha-1) - \alpha]k + b = 0 \tag{9}$$

This equation must be applied individually to the rectifying and the stripping sections. For the rectifying section: $x_o = x_d$, $x_n = x_{int}$ (the composition at the intersection of the operating lines of the rectifying and stripping sections).

$$x_{\text{int}} = \frac{x_f - b(1-q)}{1+(m-1)(1-q)} \tag{10}$$

For the stripping section:

$$\text{m} = \text{Rs}/(\text{Rs}-1) \tag{11}$$

$$\begin{aligned}\text{Rs} &= \text{L}_s/\text{B} = (\text{L}+\text{qF})/\text{B} = (\text{L}+\text{q}(\text{D}+\text{B}))/\text{B} \\ &= (\text{R}+\text{q})\text{D}/\text{B} + \text{q} = (\text{R}+\text{q})(\text{x}_\text{f} - x_b)/(x_d - x_f) + q\end{aligned} \tag{12}$$

$$b = x_b/(R_s - 1) \tag{13}$$

$$\text{x}_\text{o} = x_{\text{int}} \tag{14}$$

$$x_n = x_b \tag{15}$$

q is the feed condition (=1 for a saturated liquid, and =0 for a saturated vapor), x_f is the concentration in the feed, x_b that for the bottom, B and D are the molar rates for the bottoms and the distillate.

Said and Hamad (1984) noticed that if we use the other root (k_2) of Eq. (9), we get the correct answer. This means that the solution can be written in a somewhat symmetrical pattern. With few simple algebraic manipulations and using the relations,

$$c_1 c_2 = \alpha / m$$

$$c_1 - c_2 = (\alpha-1)(k_1 - k_2)$$

we obtain such a form as:

$$N_R = \frac{\log\dfrac{(x_o - k_1)(x_n - k_2)}{(x_o - k_2)(x_n - k_1)}}{\log\dfrac{c_2}{c_1}} \tag{16}$$

Jafarey *et al.* (1979) developed an approximate equation for binary distillation,

$$N = \frac{\log S}{\log\left(\alpha\sqrt{1-\dfrac{R+q}{(R+1)(Rx_f+q)}}\right)} \tag{17}$$

where S is the separation factor defined by the following equation:

$$S = \frac{x_d(1-x_b)}{(1-x_d)x_b} \tag{18}$$

and N is the total number of trays.

Equation (17) was obtained by simplifying the solution to Smoker's equation. It is particularly useful in computer process control applications.

The solutions of the quadratic Eq. (9) are given by

$$k_i = \frac{-(m+b(\alpha-1)-\alpha) \pm \sqrt{(m+b(\alpha-1)-\alpha)^2 - 4mb(\alpha-1)}}{2m(\alpha-1)} \tag{19}$$

For sharp separation, we can define a small parameter ε such that:

$$\varepsilon = 1 - x_d \tag{20}$$

Thus, from Eqs. (4) and (20), we obtain:

$$b = (1-m)(1-\varepsilon) \tag{21}$$

$$k_i = \frac{1+\alpha m-2m+\varepsilon(1-m)(\alpha-1) \pm \sqrt{(\alpha m-1)^2 + 2\varepsilon(1-m)(\alpha-1)(1+m\alpha)+\varepsilon^2(1-m)^2(\alpha-1)^2}}{2m(\alpha-1)} \tag{22}$$

Expanding the term under the square root for small ε to the first degree of ε, we obtain:

$$k_i = \frac{1+\alpha m-2m+\varepsilon(1-m)(\alpha-1) \pm (\alpha m-1)\left(1+\frac{\varepsilon(1-m)(\alpha-1)(1+m\alpha)}{(\alpha m-1)^2}+....\right)}{2m(\alpha-1)} \tag{23}$$

Taking the negative sign of ±, we obtain:

$$k_1 \cong \frac{(1-m)}{m(\alpha-1)} \cong \frac{1}{R(\alpha-1)} \tag{24}$$

to a zero degree in ε.

Taking the positive sign of ±, we obtain:

$$k_2 \cong 1+\varepsilon\frac{\alpha(1-m)}{(\alpha m-1)} = 1+\varepsilon\frac{\alpha}{(R(\alpha-1)-1)} \tag{25}$$

Thus,

$$k_2 - x_d \cong (1-x_d)\frac{(R+1)(\alpha-1)}{(R(\alpha-1)-1)} \tag{26}$$

The main difference between this derivation and Jafarey's *et al.* (1979) is that they used the very crude approximation;

$$k_2 \cong 1$$

Carrying out the same analysis for the stripping section, and assuming x_b is the small parameter for sharp separation, we obtain:

$$\bar{k}_1 = \frac{(\alpha(R_s-1)-R_s)}{R_s(\alpha-1)} \tag{27}$$

$$\bar{k}_2 = x_b\frac{1}{(R_s-\alpha(R_s-1))} \tag{28}$$

$$\bar{k}_2 - x_b = x_b\frac{(\alpha-1)(R_s-1)}{(R_s-\alpha(R_s-1))} \tag{29}$$

Jafarey et al. (1979) used the approximation:

$$\bar{k}_2 \cong 0$$

$\bar{k}_1, \bar{k}_2$ are the roots of the quadratic Eq. (9) for the stripping section.

Substituting Eqs. (24) and (25) in Eq. (16) and neglecting terms that contain ε, we obtain:

$$N_R = \frac{\log\left(\frac{x_d(1-x_{\text{int}})(R(\alpha-1)-1)^2}{(1-x_d)x_{\text{int}}(R(\alpha-1)-1/x_{\text{int}})(R+1)(\alpha-1)}\right)}{\log\left(\frac{\alpha R}{(R+1)}\right)} \tag{30}$$

Table 1. Steady state data and results for cases studied. All cases have saturated liquid feed (q=1)

Case	x_f	$[\alpha]$	N	N_f	x_d	x_b	D/F	L/F	N/N_{min}	R/R_{min}	**This Work** ***N***	**Jafarey** ***N***	**Gilliland** ***N***
A	0.5	1.5	40	21	0.99	0.01	.5	2.706	1.76	1.388	41.12	37.02	40.57
B	0.1	1.5	40	21	0.98	.005	.092	2.329	1.76	1.301	41.16	38.47	41.53
C	0.5	1.5	37	30	0.9	.002	.555	2.737	1.93	1.645	42.02	35.73	33.09
D	0.65	1.12	107	36	.995	0.1	.614	11.862	1.66	1.529	107.19	99.85	103.75
E	0.2	5	14	4	.9999	0.05	.158	0.226	1.99	1.144	17.31	14.17	19.39
F	0.5	1.5	10	6	.9999	.0001	.5	0.227	1.47	3.183	10.04	9.88	13.15
G	0.5	1.5	80	40	.9999	.0001	.5	2.635	1.76	1.318	79.9	75.32	84.69

Similarly we substitute Eqs. (28) and (29) in the corresponding Eq. (16) for the stripping section to obtain an expression for the number of plates in the stripping section N_S,

$$N_S = \frac{\log\left(\dfrac{x_{\text{int}}(1-x_b)(R_S(\alpha-1)-\alpha)^2}{(1-x_{\text{int}})x_b(R_S(\alpha-1)-\alpha/(1-x_{\text{int}}))(R_S-1)(\alpha-1)}\right)}{\log\left(\dfrac{\alpha(R_S-1)}{R_S}\right)}$$

$$= \frac{\log\left(\dfrac{x_{\text{int}}(1-x_b)(R_S(\alpha-1)-\alpha)^2}{(1-x_{\text{int}})x_b(R_S(\alpha-1)-\alpha/(1-x_{\text{int}}))(R_S-1)(\alpha-1)}\right)}{\log\left(\dfrac{\alpha((R+1)x_f+q-1)}{(Rx_f+q)}\right)} \tag{31}$$

Assuming $N_R \cong N_S \cong N/2$, we combine Eqs. (30) and (31) to obtain:

$$N = \frac{\log S + \log AR}{\log\left(\alpha\sqrt{1-\dfrac{R+q}{(R+1)(Rx_f+q)}}\right)} \tag{32}$$

where

$$AR = \frac{(R_S(\alpha-1)-\alpha)^2(R(\alpha-1)-1)^2}{(R_S(\alpha-1)-\alpha/(1-x_{\text{int}}))(R(\alpha-1)-1/x_{\text{int}})(R_S-1)(R+1)(\alpha-1)^2}$$

The assumption that $N_R \cong N_S \cong N/2$ is only used in combining Eqs. (30) and (31) and is justified on the basis that:

$\dfrac{\alpha R}{(R+1)}$ is not much different from $\dfrac{\alpha(R_S-1)}{R_S}$,

x_{int} is obtained from Eq. (10).

Numerical Results

Table 1 gives input data for the examples treated by Skogestad and Morari (1987). Column 4 gives the theoretical number of plates obtained from Smoker equation. The table also gives the results obtained from applying Eq. (32) derived in this paper, Eq. (17) of Jafarey *et al.*, and Eq. (1) expressing Gilliland graphs.

Equation (32) is superior to other equations, except for cases C and E for which the main assumptions for the validity of the perturbation analysis are violated. Case C represents a case for which the separation is not sharp. Case E represents a case for which the relative volatility is large. In case A, Gilliland correlation is slightly better than the present work.

Conclusions

Equation (32) represents an improvement over Eq. (17) due to Jafarey's *et al.* (1979). It gives very accurate predictions for the number of stages for a sharp distillation of binary mixtures with low constant relative volatility. Extension to multi-component distillation can be carried out using the concept of light key and heavy key components.

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J. King Saud Univ., Vol. 21, *Eng. Sci*. (1), Riyadh (2009/1430H.)

طريقة مختصرة لتصميم برج تقطيرلخليط ثنائي

مصطفى علي سليمان

قسم الهندسة الكيميائية ، كلية الهندسة ، جامعة الملك سعود
ص.ب. ٨٠٠ الرياض ١١٤٢١
المملكة العربية السعودية
mostf34@hotmail.com

(قدم للنشر في١١/٠٤/٢٠٠٧م؛ وقبل للنشر في ١٠/٠٧/٢٠٠٧م)

ملخص البحث. اعتمادًا على الحل التحليلي لسموكر (١٩٣٨م) لبرج تقطير به خليط ثنائيي ذي تطاير نسبي ثابت، اشتق جعفري وزملائه (١٩٧٩م) معادلة تصميم مبسطة لعدد الصواني النظري وقد تم إدخال بعض التعديلات على هذه المعادلة لتحسين نتائجها، وهذه المعادلة المعدلة مفيدة في تطبيقات التحكم لأنها تعطي معادلة لمعامل الفصل لا تعتمد على خصائص المادة الخارجة من برج التقطير.