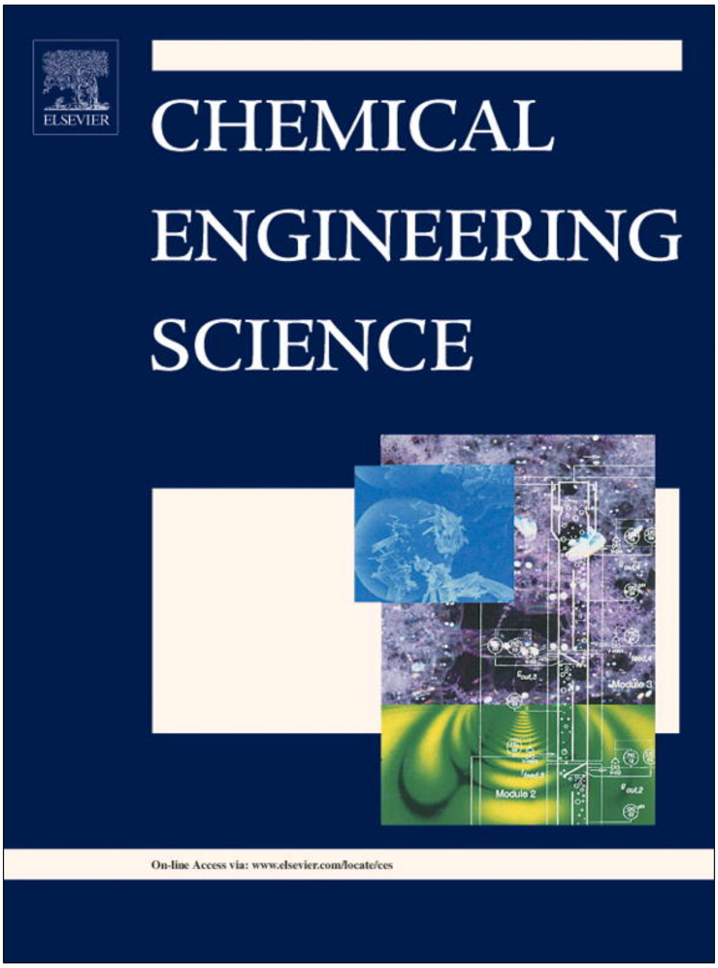

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Exponential functional rigorous method for calculation of the number of theoretical plates in distillation column

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HIGHLIGHTS

- ▸ The exponential functional rigorous method for theoretical plates number is proposed.
- ▸ The number of theoretical plates can be obtained without stepwise calculations.
- ▸ The physical significances of the model parameters are analyzed systematically.
- ▸ The model accuracy agrees well with plate-to-plate calculations and Gilliland method.

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ABSTRACT

An exponential functional rigorous calculation (EFRC) method for calculation of the number of theoretical plates in distillation column with the ideal system is proposed. In this method, the complex non-liner function describing the relation between the liquid compositions of arbitrary two theoretical plates is converted into the exponential function. For the sake of the linearization feature of the exponential function in logarithmic coordinates, the number of theoretical plates, feed location and gas or liquid composition of any theoretical plate can be obtained without stepwise plate-to-plate calculations. It can greatly help to improve the efficiency and accuracy of distillation design. And the new model is easier to be solved than Lewis method or Smoker method. The physical significances of the parameters in the EFRC model are analyzed considering the effects of the reflux ratio, relative volatility and feed phase condition, especially for that at limiting conditions. The new method can be applied to distillation design and rating, and is generalized from binary ideal system to multiple one. The EFRC method has been validated. The results indicate that the accuracy of the new method agrees well with that of the plate-to-plate calculations, and is better than that of Gilliland correlation.

1. Introduction

Distillation dominates separations for homogeneous mixtures in modern chemical process industries (Kunesh et al., 1995). It plays an irreplaceable role in the pretreatment of the feed and the separation of the production and intermediate production. It is an essential assignment to determine the number of theoretical plates, N_T, in a distillation column for a given separation. The conventional methods carrying out such calculations can be classified into two categories: rigorous calculation and shortcut one (Seader and Henley, 1998).The rigorous calculations include: the plate-to-plate calculation method, the graphical calculation method and the analytical method (Pradeep, 1985). Hence, it is quite laborious and time-consuming for the plate-to-plate calculations, where the gas/liquid compositions of each plate should be calculated stepwise from top to bottom. McCabe–Thiele method (1925) is a classic graphical method, which has the same principle as the plate-to-plate calculations. Furthermore, the boundary value method (Doherty and Malone, 2001) is a geometric one for mixtures with more than two components. It used as a triangular diagram to represent the compositions, which makes it more suitable for ternary mixtures because of its visualization.

The analytical method is an algebraic one, represented by Lewis method (1922) and Smoker method (1938). In Lewis method (1922), assuming that the liquid composition varies continuously along the height inside the tower, the number of theoretical plates were obtained by calculating the liquid composition of arbitrary two adjacent theoretical plates. It was derived

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by combining the operating line equations and equilibrium equation simultaneously. Its procedure is somewhat complex. Said (1980) simplified the Lewis equation at finite reflux by taking arithmetic average of two values of N_T, one value was calculated with respect to x_{n+1} and x_n, the other to x_n and x_{n-1}.

In Smoker method (1938), one of the intersections of the operating line and equilibrium one, $k_1(0\Delta k_1\Delta 1)$, was introduced as the model parameter. And the coordinate transform was applied, with the coordinate of k_1 defined as (0,0). In the new coordinate system, the liquid composition of any theoretical plate, x_i' ($1\le i\le n$, from top to bottom), was calculated by McCabe–Thiele method (1925). The formulas of x_i' for all theoretical plates were similar. Based on their common characteristics, the general expression of x_i' was induced, as well as the equation of N_T. In this approach, the expression of k_1 is relatively complex, and N_T is not the explicit function of the operating variables.

Strangio and Treybal (1974) deduced the simplified form of the Smoker equation by the algebraic transformation of two intersections of the operating line and equilibrium one, k_1 and k_2. Although its form is simpler than the Smoker one, the workload is equivalent, because both k_1 and k_2 have to be solved. N_T in this equation still cannot be expressed as the explicit function of the operating variables. Another simplified solution of the Smoker equation, namely JDM equation, was presented by considering the simple roots of operating line equations and equilibrium one at $x_O=1.0$ and $x_W=0.0$ (Jafarey et al., 1979; Douglas et al., 1979). x_O and x_W are the overhead and bottom product compositions (mol%), respectively. However, it has less accuracy when x_O and x_W deviate far from these assumed compositions.

The approximate solutions of the JDM equation for distillation rating and operating were brought forward by Tolliver and Waggoner (1982). Then, the JDM equation has been improved by taking into account the effects of actual compositions on the slop of the operating lines (Ma et al., 1991, 1993, 1994). In this method, two empirical constants, C and E, were introduced, which make part of the equilibrium line become straight one. Thus, the calculations of k_1 and k_2 were simplified. Its accuracy is equivalent to the Smoker method (1938) for $R/R_{min}=1.05$–1.3, where R/R_{min} is the ratio of the reflux to minimum reflux. Yet its precision is still lower when the composition deviated from $x_O=1.0$ and $x_W=0.0$.

Although the number of theoretical plates can be obtained directly without stepwise calculations in Lewis method (1922) and Smoker method (1938), it is difficult to solve these equations, and the accuracy of those simplified solutions are relative low.

Furthermore, there are several shortcut approaches for calculation of N_T, e.g., the Fenske–Underwood–Gilliland method (Fenske, 1932; Underwood, 1948; Gilliland, 1940), finite difference method (Mickley et al., 1957), Winn method (Winn, 1958), etc. They are empirical methods and can only be used to estimate N_T despite its convenience (Guerreri, 1969). In addition, the collocation approach (Stewart et al., 1985, 1986) is an algebraic approximation method considering the enthalpy balance, while the experiential object function equation and constraint condition equation of this approach should be deduced from the current industrial data and may be not convenient to get. At present, the most common rigorous approach for calculation of the number of theoretical plates is the plate-to-plate calculation method.

In this work, a new exponential function is constructed to simplify the equation form for its linearization feature in logarithmic coordinate. Therefore, an exponential functional rigorous calculation (EFRC) method for numeration of the number of theoretical plates is put forward to convert the complex nonliner function, describing the relation between the liquid compositions of arbitrary two theoretical plates, into the exponential function.

2. Exponential functional rigorous calculation (EFRC) method

2.1. Construction of exponential function

Assuming the ideal system and constant molar overflow, the operating line equation is expressed as following based on the material balance:

$$y_{i+1}=ax_i+b \tag{1}$$

with $a=R/(R+1)$ and $b=x_O/(R+1)$ (in rectifying section) or $a=\frac{L+qF}{L+qF-W}$ and $b=-\frac{Wx_W}{L+qF-W}$ (in stripping section). The subscript i ($1\le i\le n$) is the number of arbitrary theoretical plates in a section of tower. F, L, q, R, and W are the feed flow rate (kmol/h), the liquid flow rate in rectifying section (kmol/h), the feed phase condition, the reflux ratio, and the bottom product flow rate (kmol/h), respectively.

The equilibrium equation can be expressed as:

$$y_{i+1}=\frac{\alpha x_{i+1}}{1+(\alpha-1)x_{i+1}} \tag{2}$$

Combination of Eq. (1) and Eq. (2) gives:

$$x_{i+1}=\frac{Ax_i+B}{Cx_i+D} \tag{3}$$

where $A=R$, $B=x_O$, $C=R(1-\alpha)$, and $D=(1-\alpha)x_O+\alpha(R+1)$ (in rectifying section), or $A=L+qF$, $B=-Wx_w$, $C=(L+qF)(1-\alpha)$, and $D=\alpha(L+qF-W)+Wx_w(\alpha-1)$ (in stripping section).

Eq. (3) relates the liquid compositions (x_i and x_{i+1}) of two adjacent theoretical-plates. However, it is a nonlinear equation. In order to derive the analytical formula for N_T, it is necessary to convert Eq. (3) into an exponential function by introducing a new function, $Z=f(x)$, where Z monotonically corresponds to x. Z_i should be related to Z_{i+1} by the following equation so as to maintain their exponential relationship:

$$Z_{i+1}=KZ_i \tag{4}$$

where K is a constant. Similarly, we obtain:

$$Z_n=K^{(n-1)}Z_1 \tag{5}$$

Under the above-mentioned conditions, the principle of our EFRC method can be shown in Fig. 1.

In order to transform the nonlinear relationship between x_i and x_j ($i\ne j$) into a linear exponential function between Z_i and Z_j, the function Z is expressed as

$$Z_i=\frac{x_i+U}{x_i+V} \tag{6}$$

where U and V are constants and $U\ne V$ (if $U=V$, then $Z=1$). We can thus obtain from Eqs. (3) and (6) (note that Eq. 6 can be

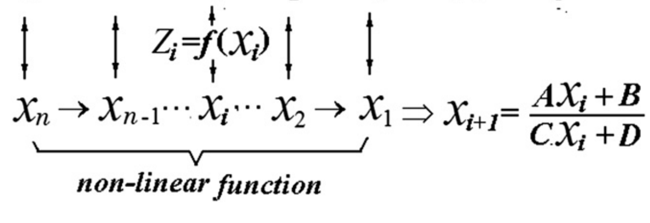

Fig. 1

rewritten as $Z_{i+1}=\frac{x_{i+1}+U}{x_{i+1}+V}$):

$$Z_{i+1}=\frac{((Ax_i+B)/(Cx_i+D)+U)}{((Ax_i+B)/(Cx_i+D)+V)}=\left(\frac{A+UC}{A+VC}\right)\left(\frac{(x_i+(B+UD)/(A+UC))}{(x_i+(B+VD)/(A+VC))}\right) \tag{7}$$

Substitution of Eq. (6) in Eq. (4) yields:

$$\frac{x_{i+1}+U}{x_{i+1}+V}=K\frac{x_i+U}{x_i+V} \tag{8}$$

For the exponential relationship between Z_i and Z_j to hold, the model parameters U, V, and K must satisfy:

$$U=\frac{B+UD}{A+UC}\ \textit{and}\ V=\frac{B+VD}{A+VC} \tag{9}$$

and

$$K=\frac{A+UC}{A+VC} \tag{10}$$

Combination of Eq. (9) and Eq. (10) yields

$$U=\frac{D-A+\sqrt{(D-A)^2+4BC}}{2C}\ \text{and}\ V=\frac{D-A-\sqrt{(D-A)^2+4BC}}{2C} \tag{11a}$$

$$K=\frac{D+A+\sqrt{(D-A)^2+4BC}}{D+A-\sqrt{(D-A)^2+4BC}} \tag{11b}$$

or

$$U=\frac{D-A-\sqrt{(D-A)^2+4BC}}{2C}\ \textit{and}\ V=\frac{D-A+\sqrt{(D-A)^2+4BC}}{2C} \tag{12a}$$

$$K=\frac{D+A-\sqrt{(D-A)^2+4BC}}{D+A+\sqrt{(D-A)^2+4BC}} \tag{12b}$$

The values of U, V, and K — which can be determined either by Eqs. (11a) and (11b) or by Eqs. (12a) and (12b) — have some influences on the value of Z_i. However, the utilization of Eqs. (11a) and (11b) instead of Eqs. (12a) and (12b) does not exert any influence on the optimum feed location and the values of N_T, x_i, and y_i. Furthermore, the relationship $(D-A)^2+4BC\geq 0$ must be maintained to ensure the existence of the exponential function described by Eq. (6) (see Appendix I).

2.2. Optimum feed location and number of theoretical plates

2.2.1. Optimum feed location

Fig. 2 shows the graphical process for optimum feed location at the gas–liquid equilibrium state ($0<q<1$). It is clear that the EFRC method uses a new definition of optimum feed location. According to the McCabe–Thiele method (1925), the concept of the optimum feed location is at the next integral theoretical plate under the intersection (x_q,y_q) of rectifying operating line and stripping one. In the EFRC method, it is at the cross section corresponding to the point (x_q,y_q) (see Fig. 2). This concept in classic plate-to-plate method is based on the fact that the mass transfer process for gas and liquid phase occurs at the theoretical plate, rather than the space between two adjacent theoretical plates. However, the concept of actual plate is different from theoretical one where the gas and liquid composition changes continuously along the tower, such as packing tower.

In EFRC method, the feed plate is divided into two parts, the portion of that above the point (x_q,y_q), is calculated by the rectifying operating line equation and its below portion by the stripping one. Obviously, it is illogical to calculate the below portion of the feed plate by rectifying operating line equation in the plate-to-plate method. Thus, the concept of feed location in the plate-to-plate calculations is less precise than the EFRC method. In this new method, the entropy increase of the feed is minimum for the least backmixing, so does the required number of theoretical plates. Besides, the concept for the optimum feed location of the EFRC method is generally applicable to other analytical methods, such as Lewis method (1922) and Smoker method (1938).

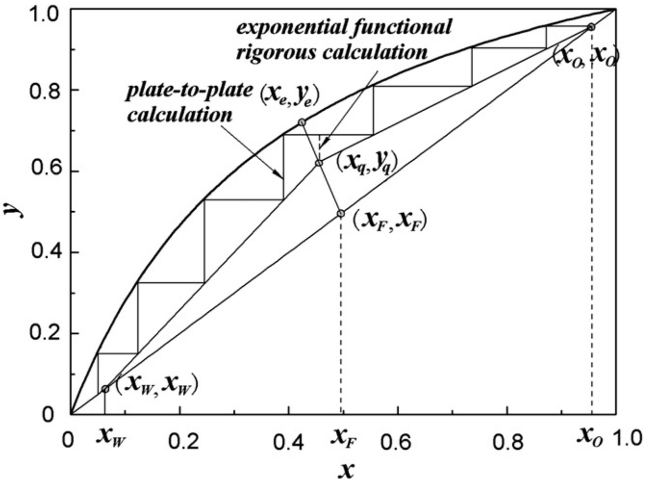

Fig. 2

2.2.2. Equations for calculation of the number of theoretical plates

The equations for calculation of the number (N) of theoretical plates in rectifying section (denoted by the subscript R) and in stripping section (denoted by the subscript S) can be derived from Eqs.(5) and (6):

$$N_R=\frac{\lg(Z_n/Z_1)}{\lg K}+1=\frac{\lg(((x_q+U)/(x_q+V))/((x_1+U)/(x_1+V)))}{\lg K}+1 \tag{13}$$

$$N_S=\frac{\lg(Z_n/Z_1)}{\lg K}=\frac{\lg(((x_W+U)/(x_W+V))/((x_q+U)/(x_q+V)))}{\lg K} \tag{14}$$

In rectifying section, the values of Z_1 and Z_n can be calculated from the liquid compositions at the top plate (x_1) and at the feed location (x_q, from top to bottom). Similarly, in stripping section, the values of Z_1 and Z_n can be calculated from x_q and x_W, respectively. The calculation process is shown in Fig. 3. In addition, the liquid compositions of the rest theoretical plates (x_j) can be readily determined by substitution of x_i into the above-mentioned equations.

It should be noted that the EFRC method uses the endpoint compositions in tower section as the boundary conditions. Therefore, the number of the theoretical plates corresponding to the feed position or to the side-draw position is double-counted in sectional calculations. Consequently, the number of the theoretical plates in Eq. (14) should be subtracted by 1, comparing to that in Eq. (13). In addition, this should be considered in sectional calculations in light of any other analytical methods, such as the Lewis method (1922), the Smoker method (1938), and the Fenske equation (1932).

3. Characteristics of the model parameters

Eqs. (11a,11b) and (12a,12b) show that the values of U, V, and K are related to the reflux ratio (R), the feed phase condition (q), and the relativity volatility (α). Therefore, in this section the effects of these operation conditions on the characteristics of U, V, and K are systemically investigated. Our analysis mainly focuses on the reflux ratio, as it is the most commonly used parameter.

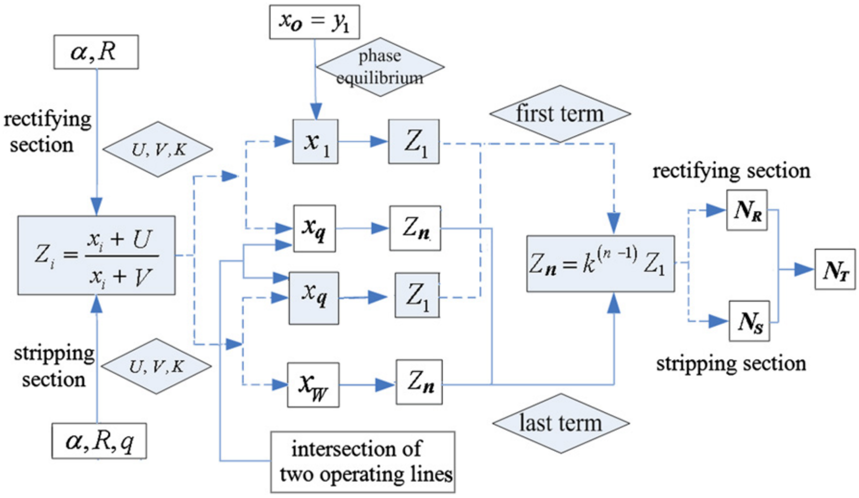

Fig. 3

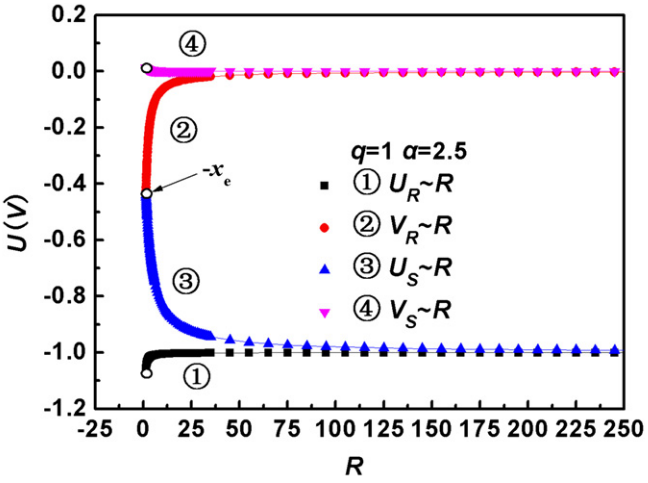

Fig. 4

3.1. Effect of reflux ratio

For convenience, the analysis has been made under the condition of x_F=44.0%, x_O=97.4%, and x_W=2.35%, where x_F is the feed composition (mol%). In addition, the values of U, V, and K are calculated from Eqs. (11a) and (11b). The thus-obtained U–R and V–R curves at $q=1$ and $\alpha=2.5$ are shown in Fig. 4. It is clear that both U_R and V_R increase monotonously with increasing R. However, the opposite trends are observed for U_S and V_S.

3.1.1. Total reflux

At total reflux, $R \to \infty$, $\lim_{R \to \infty}(R/R+1)=1$, and the rectifying operating line and the stripping one are coincided with the diagonal line in y–x equilibrium diagram. Under these conditions, Eqs. (1), (11a), (11b), (12a) and (12b) can be rewritten as:

$$y_{i+1} = x_i \tag{15}$$

$$U=-1,\ V=0,\ and\ K=\alpha \tag{16}$$

and

$$U=0,\ V=-1,\ and\ K=\frac{1}{\alpha} \tag{17}$$

At the same time, Eqs. (13) and (14) can be rewritten as:

$$N_{R,min} = \frac{\lg(Z_n/Z_1)}{\lg K} + 1 = \frac{\lg(((x_q-1)/(x_q))/((x_1-1)/(x_1)))}{\lg\alpha} + 1 = \frac{\lg(((x_1)/(1-x_1))/((x_q)/(1-x_q)))}{\lg\alpha} + 1 \tag{18}$$

$$N_{S,min} = \frac{\lg(Z_n/Z_1)}{\lg K} = \frac{\lg(((x_W-1)/(x_W))/((x_q-1)/(x_q)))}{\lg\alpha} = \frac{\lg(((x_q)/(1-x_q))/((x_W)/(1-x_W)))}{\lg\alpha} \tag{19}$$

It is now evident that Eqs. (18) and (19) are exactly the Fenske equations that were proposed by Fenske (1932) for calculation of the minimum number of theoretical plates (N_{min}) at total reflux in plate-to-plate calculations method:

$$N_{R,min} = \frac{\lg[((y_1)/(1-y_1))/((x_q)/(1-x_q))]}{\lg\alpha} = \frac{\lg[(\alpha(x_1)/(1-x_1))/((x_q)/(1-x_q))]}{\lg\alpha} = \frac{\lg[((x_1)/(1-x_1))/((x_q)/(1-x_q))]}{\lg\alpha} + 1 \tag{20}$$

$$N_{S,min} = \frac{\lg[((y_q)/(1-y_q))/((x_W)/(1-x_W))]}{\lg\alpha} - 1 = \frac{\lg[(\alpha(x_q)/(1-x_q))/((x_W)/(1-x_W))]}{\lg\alpha} - 1 = \frac{\lg(((x_q)/(1-x_q))/((x_W)/(1-x_W)))}{\lg\alpha} \tag{21}$$

This verifies the reliability of the EFRC model at total reflux, at least to some extent.

3.1.2. Minimum reflux

The minimum reflux ratio of binary systems is given by:

$$R_{min} = \frac{x_O - y_e}{y_e - x_e} \tag{22}$$

where x_e and y_e are the liquid and gas compositions (mol%) at the intersection of q line and equilibrium one, respectively.

Eq. (2) can be modified as:

$$x_e = \frac{y_e}{[\alpha-(\alpha-1)y_e]} \tag{23}$$

3.1.2.1. Rectifying section. It follows from Eqs. (11a) and (11b) that:

$$U_R+V_R=\frac{D-A}{C} \tag{24}$$

Substitution of Eq. (22) and Eq. (23) in Eq. (24) yields (see Appendix II):

$$U_R+V_R=\frac{x_o(y_e-1)}{x_o-y_e}-x_e \tag{25}$$

Similarly, we can obtain:

$$U_R-V_R=\frac{\sqrt{(D-A)^2+4BC}}{C} \tag{26}$$

Eq. (2) can be rewritten as:

$$(1-\alpha)=\frac{x_e-y_e}{x_e(1-y_e)} \tag{27}$$

Substitution of Eqs. (22), (23) and (27) in Eq. (26) gives (see Appendix III):

$$U_R-V_R=\frac{x_o(y_e-1)}{x_o-y_e}+x_e \tag{28}$$

Combining Eq. (25) with Eq. (28) gives:

$$U_R=\frac{x_o(y_e-1)}{x_o-y_e} \text{ and } V_R=-x_e \tag{29}$$

3.1.2.2. Stripping section. It can be obtained from Eqs. (12a) and (12b) that (see Appendix IV):

$$U_s+V_s=\frac{D-A}{C}=-1+\frac{1-x_W}{R(O/W)+q(F/W)}+\frac{1}{(\alpha-1)(R(O/W)+q(F/W))} \tag{30}$$

The equation of the feed phase condition, namely q line equation, can be expressed as:

$$y=\frac{q}{q-1}x-\frac{x_F}{q-1} \tag{31}$$

Substitute the intersection of the equilibrium line and operating line, (x_e, y_e), in Eq. (31) and the equilibrium equation yield:

$$q=\frac{y_e-x_F}{y_e-x_e} \tag{32}$$

There follows from Eqs. (22), (27), (30), (32) and the overall material balance ($\frac{O}{W}=\frac{x_F-x_W}{x_O-x_F}$ and $\frac{F}{W}=\frac{x_O-x_W}{x_O-x_F}$) that (see Appendix V):

$$U_S+V_S=\frac{x_W(1-y_e)}{y_e-x_W}-x_e \tag{33}$$

Similarly, we can obtain:

$$U_S-V_S=\frac{\sqrt{(D-A)^2+4BC}}{C} \tag{34}$$

Substitution of Eqs. (22), (23) and (27) in Eq. (34) gives (see Appendix VI):

$$U_S-V_S=\frac{x_W(y_e-1)}{x_W-y_e}-x_e \tag{35}$$

Combination of Eq. (33) with Eq. (35) gives:

$$U_S=-x_e \text{ and } V_S=\frac{x_W(y_e-1)}{x_W-y_e} \tag{36}$$

3.1.2.3. Brief summary. It can be demonstrated that, according to Eq. (29) and Eq. (36), $U_S=V_R=-x_e$ and both U_R and V_S are merely the function of y_e at minimum reflux ratio.

Furthermore, if $\alpha=1$, then $y_e=x_e=x_F$, therefore $U_R=(x_O(x_F-1))/(x_O-x_F)$,$V_S=(x_W(1-x_F))/(x_F-x_W)$, $U_S=V_R=-x_F$, $K_R=K_S=1.0$ at any q regardless its value.

Table 1 shows the values of U, V, and K at R_{min} and a given composition (i.e., x_F=44.0%, x_O=97.4%, and x_W=2.35%, mol%). These results provide typical examples in favor of the above-mentioned deductions.

3.2. Effect of feed phase condition

It can be seen from Eqs. (3), (11a), (11b), (12a) and (12b) that, the feed phase condition, q, exerts its influence on the model parameters in stripping section, but not in rectifying section. Fig. 5 shows the variations of U_S and V_S with R, where $\alpha=2.5$ and q increases from -0.5 to 1.5. It is evident that, if R is kept constant, then both U_S and V_S progressively decrease with increasing q. In all cases the values of U_S and V_S diminish with increasing R and approach -1.0 and 0.0, respectively, as R converges towards total reflux.

3.3. Effect of relative volatility

As can be seen from Fig. 6, the radians of the U–R and V–R curves decrease with increasing α. Therefore, the vertical variations of U and V with R are expected as $\alpha\to+\infty$. The values of $U_{\alpha=1}$ and $V_{\alpha=1}$ at R_{min} have been given in Section 3.1.

4. Model validation

In this section, the EFRC model was checked by comparisons with the plate-to-plate calculation (Guerreri, 1969) and the Gilliland correlation (Eduljee, 1975). A continuous process for separation of the benzene+toluene system at atmospheric pressure was used in comparisons. We know that x_F=75.0% (mol%), x_O=99.9%, x_W=0.1%, and α=2.54. The values of R and q are shown in Table 2. The three approaches were used to calculate N_T.

In this study, the absolute difference between the evaluated method- and the plate-to-plate results is defined as:

$$\Delta N_T=N_{T,\text{ evaluated method}}-N_{T,\text{ plate-to-plate}} \tag{37}$$

where $N_{T,\,\textbf{evaluated method}}$ is the result of the EFRC method or the Gilliland correlation ($N_{T,\,\textbf{EFRC}}$ or $N_{T,\,\textbf{Gilliland}}$), and $N_{T,\,\textbf{plate-to-plate}}$ is that of the plate-to-plate calculations. The detailed results are shown in Table 2. It can be seen that the results of the EFRC method agree well with those of the plate-to-plate calculations, and are much better than those of the Gilliland correlation (Eduljee, 1975).

5. Conclusions

An analytical method for calculation of the number of theoretical plates in distillation column with the ideal system is proposed. The number of theoretical plates, the feed location and the gas or liquid composition of arbitrary theoretical plate can be determined directly and conveniently without the use of stepwise plate-to-plate calculations. This model is easier to be solved than Lewis method or Smoker method. The plate-to-plate calculations can be replaced by the EFRC method in any

Table 1
Model parameters of the EFRC method at minimum reflux ratio (x_F=44.0%,x_O=97.4%, x_W=2.35%, mol%).

q	α	U_R	V_R	U_S	V_S	K_R	K_S	x_e	y_e
−0.5	1	−1.021	−0.4400	−0.4400	0.03160	1.000	1.000	0.4400	0.4400
	2.5	−1.015	−0.1791	−0.1797	0.0460	1.988	1.364	0.1791	0.3530
0.0	1	−1.021	−0.4400	−0.4400	0.03160	1.000	1.000	0.4400	0.4400
	1.05	−1.021	−0.4280	−0.4280	0.03160	1.029	1.023	0.4280	0.4400
	1.2	−1.021	−0.3957	−0.3957	0.03160	1.116	1.086	0.3957	0.4400
	1.5	−1.021	−0.3438	−0.3438	0.03160	1.289	1.191	0.3438	0.4400
	2	−1.021	−0.2821	−0.2821	0.03160	1.577	1.324	0.2821	0.4400
	2.5	−1.021	−0.2391	−0.2391	0.03160	1.864	1.426	0.2391	0.4400
	3	−1.021	−0.2075	−0.2075	0.03160	2.150	1.511	0.2075	0.4400
	3.5	−1.021	−0.1833	−0.1833	0.03160	2.437	1.583	0.1833	0.4400
	4	−1.021	−0.1642	−0.1642	0.03160	2.723	1.649	0.1642	0.4400
	4.5	−1.021	−0.1486	−0.1486	0.03160	3.009	1.709	0.1486	0.4400
	5	−1.021	−0.1358	−0.1358	0.03160	3.296	1.766	0.1358	0.4400
0.5	1	−1.021	−0.4400	−0.4400	0.03160	1.000	1.000	0.4400	0.4400
	2.5	−1.034	−0.3290	−0.3290	0.02000	1.708	1.5401	0.3290	0.5508
1.0	1	−1.021	−0.4400	−0.4400	0.03160	1.000	1.000	0.4400	0.4400
	1.05	−1.023	−0.4400	−0.4400	0.03005	1.029	1.0235	0.4400	0.45205
	1.2	−1.026	−0.4400	−0.4400	0.02619	1.108	1.094	0.4400	0.48529
	1.5	−1.033	−0.4400	−0.4400	0.02085	1.243	1.233	0.4400	0.54098
	2	−1.044	−0.4400	−0.4400	0.01555	1.419	1.463	0.4400	0.61111
	2.5	−1.055	−0.4400	−0.4400	0.01240	1.556	1.691	0.4400	0.66265
	3	−1.067	−0.4400	−0.4400	0.01032	1.667	1.920	0.4400	0.70213
	3.5	−1.079	−0.4400	−0.4400	0.008828	1.761	2.147	0.4400	0.73333
	4	−1.092	−0.4400	−0.4400	0.007716	1.843	2.375	0.4400	0.75862
	4.5	−1.104	−0.4400	−0.4400	0.006853	1.915	2.602	0.4400	0.77953
	5	−1.117	−0.4400	−0.4400	0.006164	1.981	2.830	0.4400	0.7971
1.5	1	−1.021	−0.4400	−0.4400	0.03160	1.000	1.000	0.4400	0.4400
	2.5	−1.086	−0.5424	−0.5427	0.008179	1.450	1.837	0.5424	0.7478

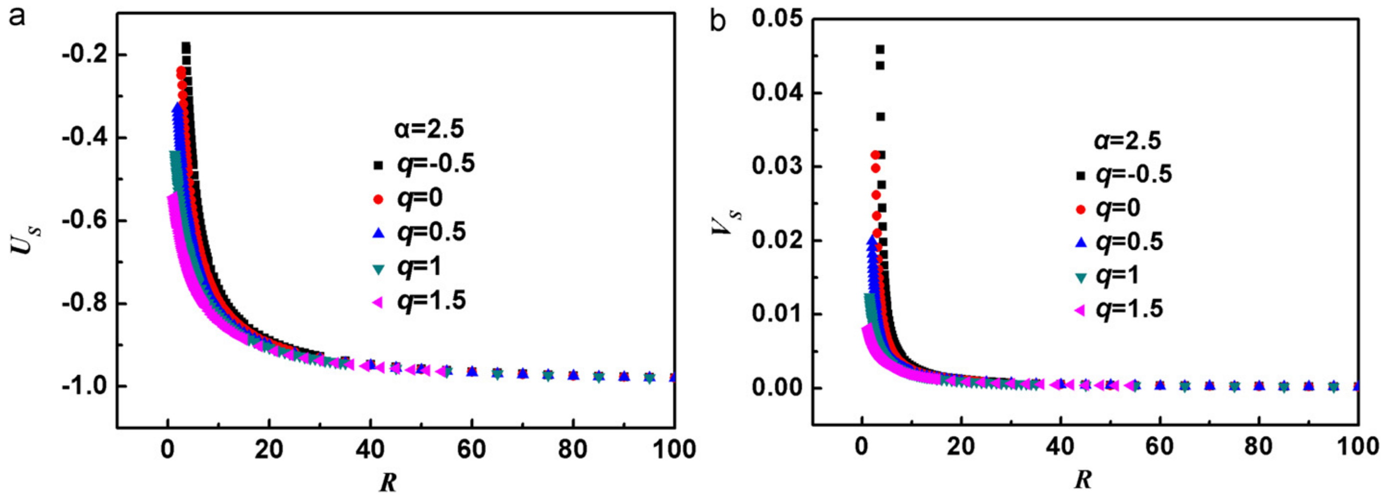

Fig. 5

application under the assumption of the ideal system and constant molar overflow. This new method can be applied to bidirectional numerical calculation since the number of theoretical plates is the explicit function of the operating variables. It is applicable for both distillation design and rating, and can be generalized from binary ideal system to multiple one. The new model has been assessed by the cited data of the plate-to-plate calculations and Gilliland correlation in this paper. It indicates that the accuracy of the EFRC method is consistent with that of the plate-to-plate calculation, and better than that of Gilliland correlation.

In the EFRC method, the cross section with the compositions of the intersection of operating lines is used as the optimum feed location (or side stream one), which distinctly defines the endpoint compositions of the section in tower. It is more reasonable than standard plate-to-plate calculation, and generally applicable to other analytical methods.

The feed location (or side stream location) is double-counted in sectional calculations in this method. The number of theoretical plates in stripping section or intermediate section should be subtracted by 1. It also must be considered in sectional calculations of any other analytical methods.

The model parameters, U_R,V_R, monotonously increase with R, while U_S,V_S monotonously decrease with R. In particular, the parameters $U=-1$, $V=0$ and $K=\alpha$,(or $U=0$, $V=-1$ and $K=1/\alpha$) at total reflux. And the formula of the EFRC model at total reflux is validated by comparison with Fenske Equation. It can be demonstrated through the derivation that U_S,V_R are equal to $-x_e$, and

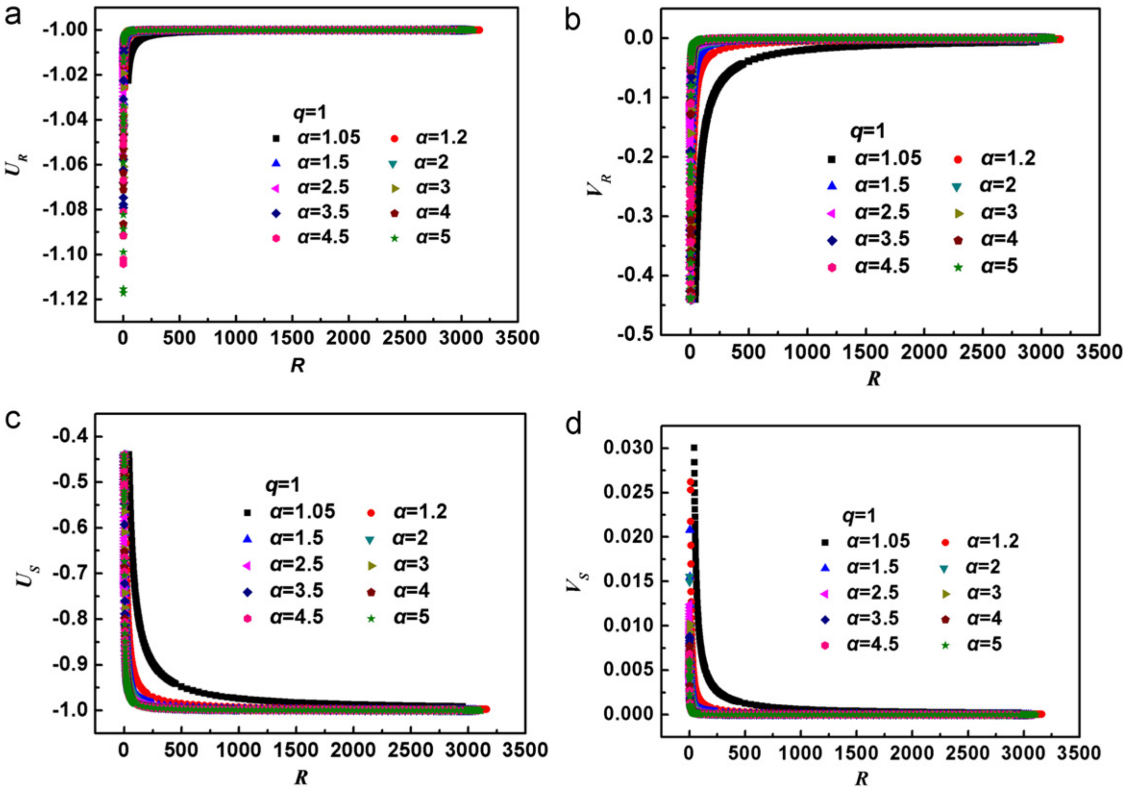

Fig. 6

Table 2
Comparisons of the results of the EFRC method, the plate-to-plate calculations, and the Gilliland correlation.

R/R_{min}	R_{min}	R	q	$N_{T,\ \text{plate-to-plate}}$	$N_{T,\ \text{EFRC}}$	ΔN_T[a]	$N_{T,\ \text{Gilliland}}$	ΔN_T[b]
1.03	0.799	0.8230	1.3	53.54	53.43	−0.11	48.89	−4.65
	0.84	0.8652	1	47.75	47.76	0.01	48.41	0.66
	0.971	1.000	0.5	44.37	44.38	0.01	48.72	4.35
	1.214	1.250	0	40.43	40.47	0.04	48.75	8.32
	1.836	1.8911	−1	35.64	35.66	0.02	48.64	13.01
1.1	0.799	0.8789	1.3	39.66	39.67	0.01	40.80	1.14
	0.84	0.9240	1	37.65	37.64	−0.01	40.32	2.67
	0.971	1.068	0.5	36.01	36.08	0.07	40.37	4.36
	1.214	1.335	0	33.64	33.62	−0.02	40.10	6.46
	1.836	2.020	−1	29.77	29.74	−0.03	39.55	9.78
1.25	0.799	0.9988	1.3	31.25	31.00	−0.25	33.61	2.36
	0.84	1.050	1	30.07	30.15	0.08	33.16	3.09
	0.971	1.214	0.5	29.60	29.60	−0.01	33.08	3.48
	1.214	1.518	0	28.08	28.10	0.02	32.70	4.62
	1.836	2.295	−1	24.99	25.05	0.06	32.02	7.03
1.4	0.799	1.119	1.3	27.32	27.27	−0.05	29.96	2.64
	0.84	1.176	1	26.74	26.74	0.00	29.55	2.81
	0.971	1.359	0.5	26.81	26.48	−0.34	29.44	2.63
	1.214	1.700	0	25.37	25.35	−0.01	29.06	3.69
	1.836	2.570	−1	22.84	22.86	0.02	28.41	5.57

[a] $\Delta N_T = N_{T,\text{ERFC}} - N_{T,\text{plate-to-plate}}$.
[b] $\Delta N_T = N_{T,\text{Gilliland}} - N_{T,\text{plate-to-plate}}$.

U_R,V_S are merely the functions of y_e at minimum reflux ratio. Furthermore, U_S and V_S at the same R decrease monotonously with q, whose effects decline with the increase of R. When R converges towards total reflux, the effect can be neglected. The greater α is, the smaller the radian of the curves are, and the sooner the values of U and V approach to constants. When α is near to infinite, the curves approach to be a rectangle. If $\alpha=1$, then U_R is merely the function of x_O, x_F; and V_S is the function of x_W, x_F at minimum reflux ratio, $U_S=V_R=-x_F$, $K_R=K_S=1.0$ at any value of q.

Nomenclature

a, b	parameter
A, B, C, D	parameter
F	feed flow rate (kmol/h)
K	parameter
L	liquid flow rate in rectifying section (kmol/h)
N_R	number of theoretical plates in rectifying section

N_S	number of theoretical plates in stripping section
N_T	total number of theoretical plates
$N_{T,min}$	minimum number of theoretical plates
O	overhead product flow rate (kmol/h)
q	feed phase condition
R	reflux ratio
R_{min}	minimum reflux ratio
U	parameter
V	parameter
W	bottom product flow rate (kmol/h)
x_O	overhead product composition (mol%)
x_e	liquid composition of intersection of q line and equilibrium line (mol%)
x_F	feed composition (mol%)
x_q	liquid composition of intersection of rectifying operating line and stripping operating line (mol%)
x_W	bottom product composition (mol%)
y_e	gas composition of intersection of q line and equilibrium line (mol%)
y_q	gas composition of intersection of rectifying operating line and stripping operating line (mol%)
Z	exponential function

Greek letters

α	relative volatility

Subscripts

e	intersection of q line and equilibrium line
F	feed
i	number of arbitrary theoretical plate
j	number of arbitrary theoretical plate, $j \neq i$
min	minimum
n	number of theoretical plate
O	overhead product
q	intersection of rectifying operating line and stripping operating line
R	rectifying section
S	stripping section
T	total column
W	bottom product

Appendix I

a. Rectifying section

$$\begin{aligned}(D-A)^2+4BC &= [(1-\alpha)x_O+\alpha(R+1)-R]^2+4x_OR(1-\alpha)\\ &= [(1-\alpha)(x_O-R-1)+1]^2+4x_OR(1-\alpha)\\ &= (1-\alpha)^2(x_O-R-1)^2+2(1-\alpha)(x_O-R-1)+1+4x_OR(1-\alpha)\end{aligned} \tag{A1}$$

Because:

$$x_O<1 \textit{ and } \alpha \geq 1 \tag{A2}$$

We obtain:

$$[(D-A)^2+4BC]\big|_{\min} > [(D-A)^2+4BC]\big|_{x_O=1} \tag{A3}$$

$$[(D-A)^2+4BC]\big|_{x_O=1} = (1-\alpha)^2R^2-2(\alpha-1)R+1 = [(\alpha-1)R-1]^2 \geq 0 \tag{A4}$$

That is:

$$[(D-A)^2+4BC]\big|_{\min} > 0 \tag{A5}$$

b. Stripping section

$$(D-A)^2+4BC = [\alpha(L+qF-W)+Wx_W(\alpha-1)-(L+qF)]^2+4Wx_W(L+qF)(\alpha-1) \geq 0 \tag{A6}$$

It follows from Eq. (A6) that:

$$(D-A)^2+4BC \geq 0 \tag{A7}$$

This demonstrates that, for an ideal system under the constant molar overflow condition, the nonlinear relationship between the liquid compositions of two arbitrary theoretical plates (x_i and x_{i+1}) can always be converted into the exponential relationship between Z_i and Z_{i+1}, where Z is an exponential function.

Appendix II

$$\begin{aligned}U_R+V_R &= \frac{(1-\alpha)x_O+\alpha(R+1)-R}{R(1-\alpha)} = \frac{(1-\alpha)x_O-(1-\alpha)R-(1-\alpha)+1}{R(1-\alpha)} = \frac{x_O-R-1}{R}+\frac{1}{R(1-\alpha)}\\ &= \frac{x_O-(x_O-y_e)/(y_e-x_e)-1}{(x_O-y_e)/(y_e-x_e)}+\frac{1}{(x_o-y_e)/(y_e-x_e)(1-\alpha)}\end{aligned}$$

$$\begin{aligned}&=\frac{(y_e-x_e)x_O-x_O+x_e}{x_O-y_e}+\frac{y_e-x_e}{(1-\alpha)(x_O-y_e)}\\&=\frac{(y_e-y_e/(\alpha-(\alpha-1)y_e))x_O-x_O+y_e/(\alpha-(\alpha-1)y_e)}{x_O-y_e}+\frac{y_e-y_e/(\alpha-(\alpha-1)y_e)}{(1-\alpha)(x_O-y_e)}\\&=\frac{y_e x_O-x_O}{x_O-y_e}+\frac{y_e-y_e x_O}{(x_O-y_e)[\alpha-(\alpha-1)y_e]}+\frac{{y_e}^2-y_e}{(x_O-y_e)[\alpha-(\alpha-1)y_e]}=\frac{x_o(y_e-1)}{x_o-y_e}-x_e\end{aligned}\tag{A8}$$

Appendix III

$$\begin{aligned}U_R-V_R&=\frac{\sqrt{[(1-\alpha)x_O+\alpha(R+1)-R]^2+4x_O R(1-\alpha)}}{R(1-\alpha)}=\frac{\sqrt{[(1-\alpha)(x_O-R-1)+1]^2+4x_O R(1-\alpha)}}{R(1-\alpha)}\\&=\frac{\sqrt{(x_O+x_O x_e-x_O y_e-x_e y_e)^2/({x_e}^2(1-y_e)^2)+4x_o(y_e-x_o)/(x_e(1-y_e))}}{(x_o-y_e)/(y_e-x_e)(x_e-y_e)/(x_e(1-y_e))}\\&=\frac{\sqrt{(x_o+x_o x_e-x_o y_e-x_e y_e)^2+4x_o x_e(1-y_e)(y_e-x_o)}}{y_e-x_o}=\frac{\sqrt{(x_o-x_o x_e-x_o y_e+x_e y_e)^2}}{y_e-x_O}=\frac{(x_o-x_o x_e-x_o y_e+x_e y_e)}{y_e-x_o}=\frac{x_o(y_e-1)}{x_o-y_e}+x_e\end{aligned}\tag{A9}$$

Appendix IV

$$\begin{aligned}U_s+V_s&=\frac{D-A}{C}=\frac{\alpha(L+qF-W)+Wx_W(\alpha-1)-(L+qF)}{(L+qF)(1-\alpha)}=\frac{(\alpha-1)(L+qF)+Wx_W(\alpha-1)-\alpha W}{(L+qF)(1-\alpha)}\\&=-1+\frac{W-Wx_W}{L+qF}-\frac{W}{(1-\alpha)(L+qF)}=-1+\frac{1-x_W}{R(O/W)+q(F/W)}+\frac{1}{(\alpha-1)\big(R(O/W)+q(F/W)\big)}\end{aligned}\tag{A10}$$

Appendix V

$$\begin{aligned}U_S+V_s&=-1+\frac{1-x_W}{(x_O-y_e)/(y_e-x_e)\,(x_F-x_W)/(x_O-x_F)+(y_e-x_F)/(y_e-x_e)\,(x_o-x_W)/(x_o-x_F)}\\&\quad+\frac{1}{(y_e-x_e)/(x_e(1-y_e))[(x_o-y_e)/(y_e-x_e)\,(x_F-x_W)/(x_O-x_F)+(y_e-x_F)/(y_e-x_e)\,(x_o-x_W)/(x_o-x_F)]}\\&=-1+\frac{(1-x_W)(y_e-x_e)(x_O-x_F)}{(x_O-y_e)(x_F-x_W)+(y_e-x_F)(x_O-x_W)}+\frac{x_e(1-y_e)(x_O-x_F)}{(x_O-y_e)(x_F-x_W)+(y_e-x_F)(x_O-x_W)}\\&=-1+\frac{(x_O-x_F)[y_e(1-x_W)+x_e(x_W-y_e)]}{(x_O-y_e)(x_F-x_W)+(y_e-x_F)(x_O-x_W)}=\frac{x_W-y_e x_W+x_e x_W-x_e y_e}{y_e-x_W}=\frac{x_W(1-y_e)}{y_e-x_W}-x_e\end{aligned}\tag{A11}$$

Appendix VI

$$\begin{aligned}U_S-V_S&=\frac{\sqrt{[(\alpha-1)(L+qF+Wx_W-W)-W]^2+4Wx_W(\alpha-1)(L+qF)}}{(1-\alpha)(L+qF)}=\frac{\sqrt{[(\alpha-1)(R(O/W)+q(F/W)+x_W-1)-1]^2+4x_W(\alpha-1)(R(O/W)+q(F/W))}}{(1-\alpha)(R(O/W)+q(F/W))}\\&=\frac{\sqrt{[(y_e-x_e)/(x_e(1-y_e))\,((x_O-y_e)/(y_e-x_e)\,(x_F-x_W)/(x_O-x_F)+(y_e-x_F)/(y_e-x_e)\,(x_O-x_W)/(x_O-x_F)\;+x_W-1)-1]^2+4x_W\,(y_e-x_e)/(x_e(1-y_e))\,((x_O-y_e)/(y_e-x_e)/(x_F-x_W)(x_O-x_F)+(y_e-x_F)/(y_e-x_e)\,(x_O-x_W)/(x_O-x_F))}}{(x_e-y_e)/(x_e(1-y_e))\,((x_O-y_e)/(y_e-x_e)\,(x_F-x_W)/(x_O-x_F)+(y_e-x_F)/(y_e-x_e)\,(x_O-x_W)/(x_O-x_F))}\\&=\frac{1/(x_e(1-y_e))\,\sqrt{(x_W+x_W x_e-x_W y_e-x_e y_e)^2+4x_W x_e(1-y_e)(y_e-x_W)}}{(x_W-y_e)/(x_e(1-y_e))}=\frac{\sqrt{(x_O-x_O x_e-x_O y_e+x_e y_e)^2}}{x_W-y_e}\\&=\frac{(x_W-x_W x_e-x_W y_e+x_e y_e)}{x_W-y_e}=\frac{x_W(1-y_e)}{x_W-y_e}-x_e\end{aligned}\tag{A12}$$

References

Doherty, M.F., Malone, M.F., 2001. Conceptual Design of Distillation Systems. McGraw-Hill Book Company, Inc., Boston/New York.

Douglas, J.M., Jafarey, A., Seemann, R., 1979. Short-cut techniques for distillation column design and control. 2. column operation and control. Ind. Eng. Chem. Process Des. Dev. 18 (2), 203–210.

Eduljee, H.E., 1975. Equations replace Gilliland plot. Hydrocarbon Process. 54 (9), 120–122.

Fenske, M.R., 1932. Fractionation of straight-run pennsylvania gasoline. Ind. Eng. Chem. 24 (5), 482–485.

Gilliland, E.R., 1940. Multicomponent rectification—estimation of the number of theoretical plates as a function of the reflux ratio. Ind. Eng. chem. 32 (9), 1220–1223.

Guerreri, G., 1969. Short-cut distillation design: beware!. Hydrocarbon Process. 48 (8), 137–142.

Jafarey, A., Douglas, J.M., McAvoy, T.J., 1979. Short-cut techniques for distillation column design and control.1. column design. Ind. Eng. Chem. Process Des. Dev. 18 (2), 197–202.

Kunesh, J.G., Kister, H.Z., Lockett, M.J., Fair, J.R., 1995. Distillation: still towering over other options. Chem. Eng. Prog. 91 (10), 43–54.

Lewis, W.K., 1922. The efficiency and design of rectifying column for binary mixture. J. Ind. Eng. chem. 14 (6), 492–496.

Ma, Y.L., Zheng, J.X., Zhou, X.H., 1991. New shortcut method for the calculation of the number of theoretical stages required in the distillation column. J. Wuhan Univ. 37 (2), 99–106, in Chinese.

Ma, Y.L., Zhou, X.H., Zheng, J.X., 1993. New method on calculation of the number of theoretical stages and feed point in the distillation column(I). J. Wuhan Univ. 39 (3), 97–102, in Chinese.

Ma, Y.L., Zhou, X.H., Zheng, J.X., 1994. A new method calculating theoretical stage number and feed point in the distillation column(II). J. Wuhan Univ. 40 (1), 85–90, in Chinese.

McCabe, W.L., Thiele, E.W., 1925. Graphical Design of Fractionating Columns. Ind. Eng. Chem. 17 (6), 605–611.

Mickley, H.S., Sherwood, T.K., Reed, C.E., 1957. Applied Mathematics in Chemical Engineering, 2nd edition McGraw-Hill Book Company, Inc., New York/Toronto/London.

Pradeep, B.D., 1985. Distillation Dynamics and Control. China Petrochemical Press, Beijing.

Said, A.S., 1980. A simple analytic formula for the number of theoretical plates in distillation. Sep. Sci. Technol. 15 (10), 1699–1708.

Seader, J.D., Henley, E.J., 1998. Separation Process Principles. John Wiley & Sons, Inc., New York/Chichester/Weinheim/Brisbane/Singapre/Toronto.

Smoker, E.H., 1938. Analytical determination of plates in fractionating columns. Trans. Am. Inst. Chem. Eng. 34 (12), 165–172.

Strangio, V.A., Treybal, R.E., 1974. Reflux-stages relations for distillation. Ind. Eng. Chem. Process Des. Dev. 13 (3), 279–285.

Stewart, W.E., Levien, K.L., Morari, M., 1985. Simulation of fractionation by orthogonal collocation. Chem. Eng. Sci. 40 (3), 409–421.

Swartz, C.L.E., Stewart, W.E., 1986. A collocation approach to distillation column design. AIChE J. 32 (11), 1832–1838.

Tolliver, T.L., Waggoner, R.C., 1982. Approximate solutions for distillation rating and operating problems using the smoker equations. Ind. Eng. Chem. Fundam. 21 (4), 422–427.

Underwood, A.J.V., 1948. Fractional distillation of multicomponent mixtures. Chem. Eng. Prog. 44 (8), 603–614.

Winn, F.W., 1958. New relative volatility method for distillation calculations. Pet. Refiner 37 (5), 216–218.