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A smoker equation based algorithm for binary distillation design calculations

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Abstract

An algorithm- based on smoker's analytical equation- suitable for the development of computer programs, for the determination of some design parameters of a binary distillation column was presented. A sample problem presented by Richardson et. al. (2003) was modified, with respect to constant relative volatility, and solved using the algorithm. We compared the solution obtained using the algorithm to that by Backhurst and Harker (1999) using McCabe-Thiele method. The deviation of 4.25% observed can be explained based on the assumption of constant relative volatility. This deviation is not only acceptable in comparison to a deviation of about 23.25% that could exist between solutions obtained using McMabe-Thiele and Fenske's method at total reflux, but also safe since it does not reduce but adds to the number of theoretical plates, thus ensuring that operational targets of purity in the product are met. Apart from suitability under normal conditions, the algorithm is suitable when concentration of more volatile component of either product is very low or relative volatility is low, conditions under which the McCabe-Thiele method is impracticable.

Keywords: Binary distillation; McCabe-Thiele method; Smoker's equation; CAD; relative volatility; Lewis-Sorrel method

1. Introduction

Distillation is agreeably the most widely applied method of separation because it has the advantage of handling a wide range of throughput, feed composition and also the ability to achieve high product purity. Binary distillation is a unit operation for separating two components in a mixture between a vapour and liquid phase based on the difference in the volatilities of the components (Sinnot, 2005; Richardson et. al., 2003). In calculating the design parameters for binary distillation, two main methods are applied. These are Lewis-Sorrel method and McCabe-Thiele method. The Lewis-Sorrel method can also be applied to multi-component distillation to determine the number of plates and is the basis of modern computerized methods for design of distillation columns (Treybal, 1982; Perry and Green, 1997; Luyben, 2008). Techniques like McCabe-Thiele method become impracticable when concentration of more volatile component of either product is very low or the volatility is low.

Alleva (1962) offered a solution to the first problem by using a log-log plot, while Robinson and Gilliland (1950) presented two equations for obtaining the number of plates for the rectifying and stripping sections. Smoker (1938) presented an analytical equation that can be used to determine the number of equilibrium stages for a distillation column operating at a nearly constant relative volatility. Though this method is suitable for any problem in which the relative volatility for the rectifying and stripping sections may be taken as being relatively constant, it is particularly useful when the relative volatility is low or concentration of more volatile component in either product is very low, thus making it robust. It thus takes care of situations when McCabe-Thiele diagram is impracticable, like the case of separation of close boiling isomers, where the relative volatility is close to unity.

Modern engineering practice is becoming largely dependent on computer and information technology due to the phenomenal growth in computer hardware. Hence the design, maintenance and operation of plants are performed using computer-aided design (CAD) (Teicholz, 1985; Cogner, 1994; Chandrapatla and Berry, 1996).

There is therefore an ever-increasing need to modify CAD techniques using methods found to be computationally efficient and robust.

2. Derivation of equations

A straight operating line can be represented by the equation;

$$y = Sx + b \tag{1}$$

In terms of relative volatility, the equilibrium values of y are given by;

$$y = \frac{\alpha\, x}{1+(\alpha-1)x} \tag{2}$$

Eliminating y from equations (1) and (2) gives a quadratic equation in x of the form;

$$S(\alpha-1)x^2 + (S+(\alpha-1)-\alpha)x + b = 0 \tag{3}$$

For any particular distillation problem, the above equation will have only one real root, k, between 0 and 1, such that;

$$S(\alpha-1)k^2 + (S+(\alpha-1)-\alpha)k + b = 0 \tag{4}$$

Where k is the value of the x co-ordinate at the point where the extended operating lines intersect with the vapour-liquid equilibrium curve. Smoker shows that the number of stages required is given by the equation;

$$Ni = \log\left(\frac{x_o^{*}(1-\beta x_n^{*})}{x_n^{*}(1-\beta x_n^{*})}\right) / \log(\alpha / S_c^{\,2}) \tag{5}$$

Where,

$$\beta = \frac{S_c(\alpha-1)}{\alpha - S_c^{\,2}} \tag{6}$$

Ni is the number of stages required to effect the separation represented by the concentration change from x_0^{*} to x_n^{*}.
Where $x_0^{*} = (x - k)$ and $x_0^{*} > x_n^{*}$.

$$c = 1+(\alpha-1)k \tag{7}$$

S = slope of the operating line
α = relative volatility, assumed constant over x_0^{*} to x_n^{*}.
For a column with a single feed and no side streams, rectifying section equations will be given as;

$$x_0^{*} = x_d - k \tag{8}$$

$$x_n^{*} = x_f - k \tag{9}$$

$$S = R/(R+1) \tag{10}$$

$$b = x_d/(R+1) \tag{11}$$

Stripping section equations will be given as;

$$x_0^{*} = x_f - k \tag{12}$$

$$x_n^{*} = x_b - k \tag{13}$$

$$S = \frac{Rx_f + x_d - (R+1)k - x_b}{(R+1)(x_f - x_b)} \tag{14}$$

$$b = \frac{(x_f - x_b)x_b}{(R+1)(x_f - x_b)} \tag{15}$$

If the feed stream is not at its boiling point, x_f - for the stripping section - is replaced by the value of x at the intersection of the operating lines;

$$x_f^{*} = \frac{b + (x_f/(q-1))}{(q/(q-1)) - S} \tag{16}$$

2.1. Algorithm for binary distillation design calculations

Input: α, R, x_d, x_f, x_b, q

Rectifying Section Calculations:

$E_{10} \rightarrow S$
$E_{11} \rightarrow b$
$E_4 \rightarrow k$, subject to 0 < k < 1
$E_8 \rightarrow x_0^{*}$
$E_9 \rightarrow x_n^{*}$
$E_7 \rightarrow c$
$E_6 \rightarrow \beta$
$E_5 \rightarrow N_R$

Stripping Section Calculations:
If feed is not at boiling point

$E_{16} \rightarrow new \quad x_f$

Else; retain x_f

$E_{14} \rightarrow S$
$E_{15} \rightarrow b$
$E_4 \rightarrow k$, subject to 0 < k < 1
$E_{12} \rightarrow x_0^{*}$
$E_{13} \rightarrow x_n^{*}$
$E_7 \rightarrow c$
$E_6 \rightarrow \beta$
$E_5 \rightarrow N_S$

Compute $N = N_R + N_S$

2.2. A sample calculation

A continuous rectifying column treats a mixture consisting of 40% of benzene by weight and 60% of toluene at the rate of 4kg/s, and separates it into a product containing 97% of benzene and a liquid containing 98% toluene. The feed is at its boiling point. If a reflux ratio of 3.5 to 1 is employed, how many plates are required in the column (Richardson et. al., 2003).

Solution

We modify the problem by using a relative volatility of 2.46 instead of the equilibrium data (Richardson et. al., 2003). This value of relative volatility closely matches with the equilibrium data.

Input: $\alpha = 2.4600$, $R = 3.5000$, $x_d = 0.9740$, $x_f = 0.4400$, $x_b = 0.0240$.

The input data were obtained by converting the values given as percentage by weight to their molar equivalents (Backhurst and Harker, 1999).

Output 1:
$S = 0.7778$
$b = 0.2164$
$k = 0.1877$
$x_0^* = 0.7863$
$x_n^* = 0.2523$
$c = 1.2740$
$\beta = 1.2081$
$N_R = 5.6512$

Output 2:
$S = 1.2853$
$b = -6.8462 \times 10^{-3}$
$k = 0.6370$
$x_0^* = -0.1970$
$x_n^* = -0.6130$
$c = 1.9300$
$\beta = -1.5560$
$N_R = 5.7736$
$N = 11.4248$

3. Discussion

Backhurst and Harker (1999) solved the same problem presented in this work using the McCabe-Thiele method and obtained the solution as ten (10) theoretical plates. In consideration that the reboiler and condenser account for one theoretical plate, the number of theoretical plates based on our algorithm becomes 10.4248 theoretical plates.The observed deviation (a deviation of 4.25%) can be explained based on the assumption of constant relative volatility and its use in place of the actual equilibrium data.

The Fenske's equation is another relation that assumes a constant relative volatility. Backhurst and Harker (1999) compared calculation of number of plates at total reflux, using both McCabe-Thiele and Fenske's equation, and concluded that a deviation (reduction in actual number of plates required) of about 23.25% was justifiable based on the assumption of constant relative volatility.

4. Conclusion

In comparison to the deviation between Fenske's equation and McCabe-Thiele method, the solution obtained using the algorithm based on Smoker's analytical equation is acceptable. It can also be observed that the deviation adds to the number of theoretical plates obtained using McCabe-Thiele method, thus ensuring the achievement of the required product purity, unlike a deviation that reduces the actual number of theoretical plates, as was the case of Fenske's equation.

Since the algorithm computes the number of plates in the rectifying and stripping sections of the column separately, it also gives an indication of the position of the feed plate. The algorithm is therefore a robust tool for binary distillation column design calculations, both under normal conditions and those of low volatility, or when concentration of more volatile component in either product is very low.

Nomenclature

Symbol	Definition	Units
E_i	Equation (i)	Nil
x	Molar fraction of more volatile component	Dimensionless
x_f	Molar fraction of more volatile component in feed	Dimensionless
x_d	Molar fraction of more volatile component in distillate	Dimensionless
x_b	Molar fraction of more volatile component in bottoms	Dimensionless
α	Relative volatility	Dimensionless
R	Reflux ratio	Dimensionless
N_R	Number of plates in the rectifying section	Dimensionless
N_S	Number of plates in the rectifying section	Dimensionless
N	Number of plates in the rectifying section	Dimensionless
q	Heat required to vapourize one mole of a component	J/mol

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