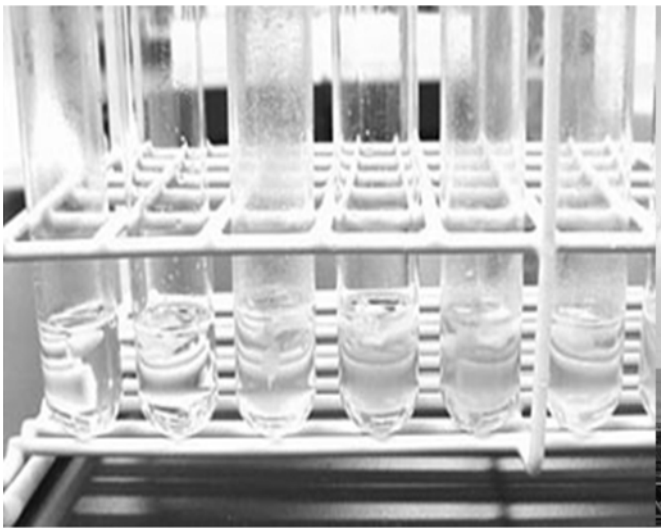
Calculation of Minimum Number of Theoretical Stages using Fenske Equation



September 2, 2010

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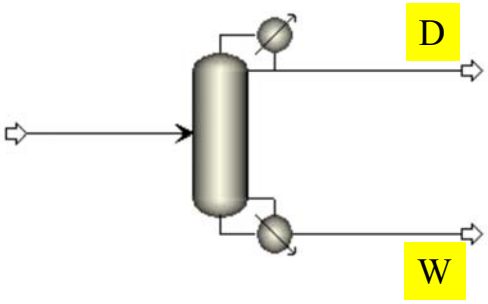
Introduction

- When performing a new distillation calculation, it is necessary to determine the theoretical number of stages (and/or the reflux ratio) after determining the operating pressure. A plotting method using the McCabe-Thiele method is also effective, but it is difficult to apply to multicomponent systems.
- On the other hand, there is a shortcut method that is often used as a guideline for multicomponent distillation calculation. In this shortcut method, the minimum number of theoretical stages and the minimum reflux ratio are obtained, and then the theoretical number of stages and the reflux ratio can be determined by using Gilliland's correlation. For systems that are not strongly non-ideal, it is an effective method to estimate rough values.
- Here, we will introduce the Fenske equation for finding the minimum number of theoretical stages.

Fenske Equation

$$N_{\min}+1=\frac{\log\left\{\left(\frac{x_{Lk,D}}{x_{Hk,D}}\right)\left(\frac{x_{Hk,W}}{x_{Lk,W}}\right)\right\}}{\log\left(\alpha_{Lk,Hk}\right)}$$

$$\alpha_{Lk,Hk}=\sqrt{\left(\frac{K_{Lk,D}}{K_{Hk,D}}\right)\left(\frac{K_{Lk,W}}{K_{Hk,W}}\right)}$$



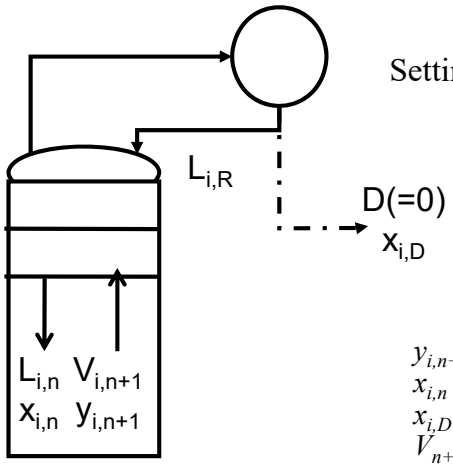
$N_{\min}$: Minimum number of theoretical stages
x_{Lk} : Light key component molar fraction
x_{Hk} : Heavy key component molar fraction
$\alpha_{Lk,Hk}$: Average relative volatility of light key component to heavy key component
K_{Lk} : Light key component vapor-liquid equilibrium constant
K_{Hk} : Heavy key component vapor-liquid equilibrium constant
Subscript $,D$: Distillate (D)
Subscript $,W$: Bottoms (W)

Fenske Equation - Derivation

The Fenske equation is a formula for finding the minimum number of theoretical stages, which means the number of theoretical stages required in the total reflux state. That is, the distillate flow rate (D) = 0.
Here, the material balance equations of the distillation column rectifying section in the state of total reflux are sorted out.

$$V_{n+1}=L_n+D$$
$$V_{n+1}y_{i,n+1}=L_nx_{i,n}+Dx_{i,D}$$

Material balance equations



Setting D=0 into the material balance equations yields:

$$V_{n+1}=L_n$$
$$V_{n+1}y_{i,n+1}=L_nx_{i,n}$$
$$\therefore y_{i,n+1}=\frac{L_n}{V_{n+1}}x_{i,n}=x_{i,n} \quad \cdots (1)$$

$y_{i,n+1}$:Vapor composition of component i rising from stage n+1
$x_{i,n}$: Liquid composition of component i falling from stage n
$x_{i,D}$: Distillate composition of component i
V_{n+1} : Vapor flow rate rising from stage n+1
L_n : Liquid flow rate falling from stage n
L_R : Reflux flow rate
D : Distillate flow rate

Fenske Equation - Derivation

Substituting the vapor-liquid equilibrium relation equation at stage *n* into Eq. 1, the following relations are obtained.

$$x_{i,n-1} = K_{i,n} x_{i,n} \qquad y_{i,n} = K_{i,n} x_{i,n}$$

Vapor-liquid equilibrium equation

The above equations hold for any component. Therefore, by applying them to components *i* and *j*, and by dividing both sides, Eq. 2 is obtained.

$$\left(\frac{x_{i,n-1}}{x_{j,n-1}}\right) = \left(\frac{K_{i,n}}{K_{j,n}}\right)\left(\frac{x_{i,n}}{x_{j,n}}\right) \qquad \ldots (2)$$

Eq. 2 is a recurrence equation, and when it is expanded it becomes Eq. 3.

$$\left(\frac{x_{i,D}}{x_{j,D}}\right) = \left(\frac{K_{i,1}}{K_{j,1}}\right)\left(\frac{K_{i,2}}{K_{j,2}}\right)\left(\frac{K_{i,3}}{K_{j,3}}\right)\cdots\left(\frac{K_{i,n-1}}{K_{j,n-1}}\right)\left(\frac{K_{i,n}}{K_{j,n}}\right)\left(\frac{x_{i,n}}{x_{j,n}}\right) \qquad \ldots (3)$$

Fenske Equation - Derivation

If the relative volatility is taken to be constant, the product of the vapor-liquid equilibrium constant ratios can be represented by relative volatility α_{ij}.

$$\left(\frac{K_{i,1}}{K_{j,1}}\right)\left(\frac{K_{i,2}}{K_{j,2}}\right)\left(\frac{K_{i,3}}{K_{j,3}}\right)\cdots\left(\frac{K_{i,n-1}}{K_{j,n-1}}\right)\left(\frac{K_{i,n}}{K_{j,n}}\right) = \alpha_{i,j}^{\,n}$$

Using the relative volatility to rearrange Eq. 3 yields Eq. 4.

$$\left(\frac{x_{i,D}}{x_{j,D}}\right) = \alpha_{i,j}^{\,n}\left(\frac{x_{i,n}}{x_{j,n}}\right) \qquad \ldots (4)$$

By considering that there is the effect of one theoretical stage at the bottom of the column (the reboiler), Eq.5 is obtained.

$$\left(\frac{x_{i,D}}{x_{j,D}}\right) = \alpha_{i,j}^{\,n+1}\left(\frac{x_{i,W}}{x_{j,W}}\right) \qquad \ldots (5)$$

Fenske Equation - Derivation

The Fenske equation is obtained by taking the logarithms of both sides of Eq. 5 and rearranging.

$$\log\left(\frac{x_{i,D}}{x_{j,D}}\right) = (n+1)\log\alpha_{i,j} + \log\left(\frac{x_{i,W}}{x_{j,W}}\right)$$

$$(n+1)\log\alpha_{i,j} = \log\left(\frac{x_{i,D}}{x_{j,D}}\right) - \log\left(\frac{x_{i,W}}{x_{j,W}}\right)$$

Fenske Equation

$$n+1 = \frac{\log\left\{\left(\frac{x_{i,D}}{x_{j,D}}\right)\left(\frac{x_{j,W}}{x_{i,W}}\right)\right\}}{\log\alpha_{i,j}} \qquad N_{\min}+1 = \frac{\log\left\{\left(\frac{x_{Lk,D}}{x_{Hk,D}}\right)\left(\frac{x_{Hk,W}}{x_{Lk,W}}\right)\right\}}{\log(\alpha_{Lk,Hk})}$$

This equation indicates that the required minimum number of theoretical stages including the reboiler is *N*min + 1, when in the total reflux condition the distillate composition is x_D and the bottom composition is x_W, and when the light key component (*Lk*) and the heavy key component (*Hk*) are applied as components *i* and j respectively.

Fenske Equation - Derivation

As is apparent from the derivation of the equation, the relative volatilities $\alpha_{i,j}$ should be used as the respective values at each stage of the distillation column.

However, in order to simplify the calculation, it is common to use a geometric average value of the relative volatilities at the top and bottom of the column.

$$\alpha_{Lk,Hk} = \sqrt{\left(\frac{K_{Lk,D}}{K_{Hk,D}}\right)\left(\frac{K_{Lk,W}}{K_{Hk,W}}\right)}$$

Relative volatility geometric average

For α_{lk}, it is normal to take the geometric average of the values at the top and bottom conditions, but when the difference between them is very large the above equation is not used. In that case, it should be based on a calculation using successive stages.

"Jyouryu Riron to Keisan" (*in Japanese*: Distillation Theory and Calculation), P.329, Kogaku-tosho

Applying the Fenske Equation

The Fenske equation is applied to the following system:
Benzene 50mol%– Toluene 40mol% –C10 Components 10mol%
Calculation is done by setting the distillate flow rate at 49.8 kmol/hr, and the overhead Benzene purity at 0.997.

Feed Light key comp	50.0	kmol/hr
Feed Heavy key comp	40.0	kmol/hr
Dist.	49.8	kmol/hr
xLkD	0.997	
xHkD	0.003	
BTM	50.2	kmol/hr
xLkW	0.007	
XHkW	0.794	
α ij=	2.43	
log ((xiD/xjD)*(xjW/xiW))	4.578686	
log α ij	0.384813	
Nmin =	10.90	

When α = 2.43, the obtained result is a minimum number of theoretical stages = 11.

On the other hand, rigorous distillation calculations including a condenser and a reboiler were performed in a process simulator with a number of 11 theoretical stages and a reflux ratio of 100.

Stage	BENZENE	TOLUENE	C10
1	0.9972	0.0028	0.0000
13	0.0067	0.7941	0.1992

Simulation Result:
Same result as Fenske Equation.

Conclusion

- The Fenske equation was found to be derived from the mass balance equations in the distillation column in the state of total reflux.
- By deriving the equation, it became clear that the relative volatilities $\alpha_{i,j}$ should be used as the respective values at each stage of the distillation column. In other words, this means that it is difficult to apply the Fenske equation if it is not used for an ideal system in which the relative volatility remains almost constant.
- The components that can be handled are limited, but if the relative volatility of the system does not significantly change, it is possible to obtain an indication of the minimum number of theoretical stages required for multicomponent distillation separation using the Fenske equation.