Minimum Reflux Ratio Calculation by Underwood Method

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Introduction

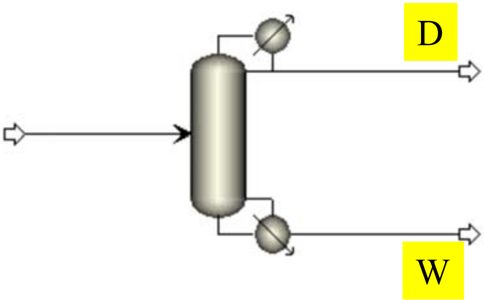
- In multicomponent distillation calculations, the approximate theoretical number of stages can be obtained when it is possible to find the minimum reflux ratio.
- Whereas for binary systems it can be easily obtained by a graphical method, elaborate calculations are required for multicomponent systems.
- Among calculation methods of the minimum reflux ratio worthy of mention are the Colburn method, the Gilliland method, the May method and the Scheibel method, but here it is the Underwood method which is the best known method that will be introduced.

Expression of Minimum Reflux Ratio by the Underwood Method

$$R_{\min} = \sum_i \left(\frac{\alpha_{1i} x_{iD}}{k - \alpha_{1i}} \right)$$

$$\sum_i \left(\frac{\alpha_{1i} x_{iF}}{k - \alpha_{1i}} \right) = -q$$

$$k = \left(1 + \frac{1}{R} \right) K_{1\infty}$$



$R_{\min}$: Minimum reflux ratio

k : This parameter is determined from the reflux ratio (R) and the equilibrium constant ($K_{1\infty}$) of component 1.

$K_{1\infty}$: Equilibrium constant of component 1 at the pinch point

x_{iF} : Feed mole fraction of component i

x_{iD} : Distillate mole fraction of component i

α_{1i} : Relative volatility of component 1 (highest volatile component) to component i

q : Preheated feed $F_{\text{liq}}/F_{\text{Total}}$

Underwood's Equations - Derivation

- Operating Line Equation:
  The operating line equation is derived from the material balance equation under the following assumptions.

1. Relative volatilities are constant in the rectifying section and the stripping section.
2. The vapor and liquid flow rates are constant (equimolar flow) in each stage.

Component material balance equation

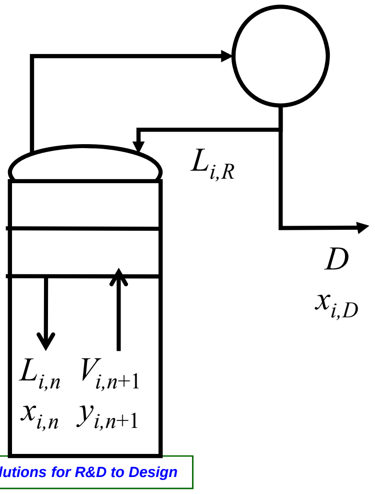
$$V_{n+1} y_{i,n+1} = L_n x_{i,n} + D x_{i,D} \quad \ldots \quad (1)$$

Rearranging for y by using assumption 2 yields

$$\boxed{\begin{aligned} y_{i,n+1} &= \frac{L}{V} x_{i,n} + \frac{D}{V} x_{i,D} \\ &= m x_{i,n} + a_i \quad \ldots \quad (2) \end{aligned}}$$

Setting $\frac{L}{V} = m$

$$\frac{D}{V} x_{i,D} = a_i$$



$y_{i,n+1}$: Vapor composition of component i rising from stage n+1

$x_{i,n}$: Liquid composition of component i descending from stage n

$x_{i,D}$: Distillate composition of component i

V : Vapor flow rate rising from stage

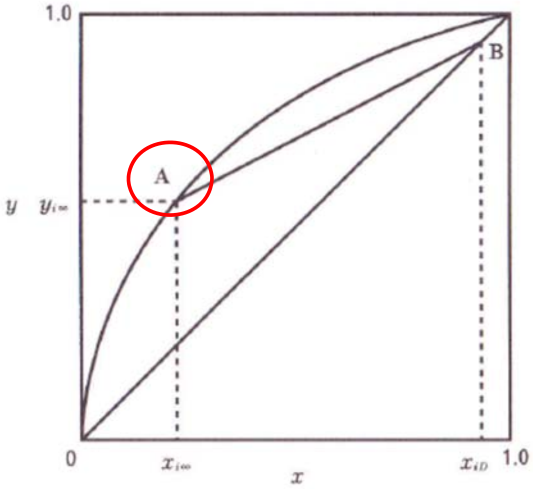
L : Liquid flow rate descending from stage

D : Distillate flow rate

Underwood’s Equations - Derivation

- The rectifying section operating line is line AB in the vapor-liquid equilibrium diagram (right figure).
- As the reflux ratio decreases, point A (the pinch point) is obtained at the intersection of the operating line and the equilibrium line. At this point an infinite number of stages is required and the composition hardly changes.
- Substituting the vapor-liquid equilibrium equation (Eq. 3) in the distillation column at stage n into Eq. 2 yields Eq. 4.

Binary Vapor-Liquid Equilibrium



$$y_{i,n} = K_{i,n} x_{i,n} \qquad \ldots (3)$$

$$K_{i,n+1} x_{i,n+1} = m x_{i,n} + a_i \qquad \ldots (4)$$

Vapor-liquid equilibrium relationship

$K_{i,n+1}$: Vapor-liquid equilibrium ratio of i component at stage n+1

Underwood’s Equations - Derivation

Since the composition hardly changes near the pinch point, Eq (5) is obtained as follows.

$$\left.\begin{aligned} x_{i,n+1} &= x_{i,n} = x_{i,\infty} \\ K_{i,n+1} &= K_{i,n} = K_{i,\infty} \end{aligned}\right\} \qquad \ldots (5)$$

Eq. 6 is obtained by substituting Eq. 5 into Eq. 4 and rearranging it.

$$K_{i,\infty} x_{i,\infty} = m x_{i,\infty} + a_i$$

$$\left(K_{i,\infty} - m\right) x_{i,\infty} = a_i$$

$$x_{i,\infty} = \frac{a_i}{K_{i,\infty} - m} \qquad \ldots (6)$$

$K_{i,\infty}$: Vapor-liquid equilibrium ratio of component i at the pinch point stage

α_{1i} : Relative volatility of component i to component 1

Eq. 7 is obtained by using the relative volatility α_{1i}.

α is assumed to be constant within the column.

$$\alpha_{1i} = \frac{K_1}{K_i}$$

$$\boxed{\begin{aligned} x_{i,\infty} &= \frac{a_i}{K_{1,\infty}/\alpha_{1i} - m} \\ &= \frac{\alpha_{1i} a_i / m}{K_{1,\infty}/m - \alpha_{1i}} \qquad \ldots (7) \end{aligned}}$$

Underwood's Equations - Derivation

Eq. 7 holds for all components in a multicomponent system, and since the sum of the compositions is 1, Eq. 8 is obtained as follows.

$$\sum_i x_{i\infty} = 1 \qquad \sum_i x_{i,\infty} = \sum_i \frac{\alpha_{1i} a_i / m}{K_{1,\infty}/m - \alpha_{1i}} = 1$$

Setting $K_{1,\infty}/m = k$

$$\frac{a_i}{m} = \frac{x_{i,D}}{R+1} \Big/ \frac{R}{R+1} = \frac{x_{i,D}}{R}$$

$$\boxed{\sum_i \frac{\alpha_{1i} x_{1D}}{k - \alpha_{1i}} = R \quad \ldots (8)}$$

Since Eq. 8 holds for any arbitrary reflux ratio, it can be expressed for both the rectifying section and the stripping section (for the stripping section the k value becomes k' and the liquid flow rate becomes *L'*).

$$\sum_i \frac{\alpha_{1i} D x_{iD}}{k - \alpha_{1i}} = L \quad \ldots (9)$$

Rectifying section

$$R = \frac{L}{D}$$

$$\sum_i \frac{\alpha_{1i} W x_{iW}}{k' - \alpha_{1i}} = -L' \quad \ldots (10)$$

Stripping section

R : Reflux ratio
W : Bottom flow rate

Underwood's Equations – Meaning of Equations

Consider the meaning of Eq. 9 and Eq. 10.

If the relative volatility, top product purity and distillate flow rate are known, since the flow is equimolar, the parameters *k* and *k'* can be obtained by setting the reflux rate *L*.

$$\sum_i \frac{\alpha_{1i} D x_{iD}}{k - \alpha_{1i}} = L \qquad k = K_{1,\infty} \Big/ \frac{R}{R+1}$$

$$\sum_i \frac{\alpha_{1i} W x_{iW}}{k' - \alpha_{1i}} = -L' \qquad = \left(1 + \frac{1}{R}\right) K_{1,\infty}$$

From the equations it can be seen that when the reflux rate is very large (*L* is large), *k* is slightly larger than *α* and *k'* is slightly smaller than *α*.

On the other hand, when reducing the reflux flow rate, *k* approaches infinity and *k'* approaches zero.

However, if the reflux is decreased beyond the point where each k is equal, the target distillate composition cannot be obtained (the composition variations no longer match in the calculations from the top and the bottom of the column). This point is the minimum reflux state ($k = k'$).

Underwood's Equations - Derivation

Assuming that the reflux rate is Lmin and the reflux ratio is Rmin in the condition where $k = k'$, the following relationship (Eq. 11) is obtained.

$$R_{\min} = \frac{L_{\min}}{D} \quad \dots (11)$$

By adding both sides of Eq. 9 and Eq. 10, Eq. 12 is obtained.

$$\sum_i \frac{\alpha_{1i} D x_{iD}}{k - \alpha_{1i}} + \sum_i \frac{\alpha_{1i} W x_{iW}}{k - \alpha_{1i}} = L - L'$$

$$\sum_i \frac{\alpha_{1i} \left(D x_{iD} + W x_{iW} \right)}{k - \alpha_{1i}} = \sum_i \frac{\alpha_{1i} F x_{iF}}{k - \alpha_{1i}} = L - L' \quad \dots (12)$$

Here, in order to obtain the relationship of L - L', consider the feed condition.

$L_{\min}$: Minimum reflux rate
$R_{\min}$: Minimum reflux ratio

Underwood's Equations – Feed Condition

For the feed stage, Eq. 13 is obtained by considering the vapor-liquid flows separately.

$$L_f = L_n + L_F$$

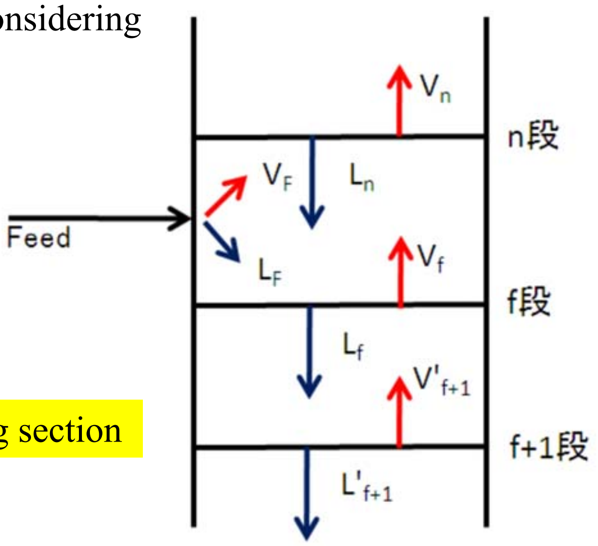
$$V_n = V_f + V_F$$

$$\text{Setting } \frac{L_f}{F} = q$$

$$\left.\begin{aligned} L_f &= L_n + qF \\ V_f &= V_n - (1-q)F \end{aligned}\right\} \text{Rectifying section}$$

$$\text{Setting } L_f = L'_{f+1},\ V_f = V'_{f+1}$$

$$\left.\begin{aligned} L'_{f+1} &= L_n + qF \\ V'_{f+1} &= V_n - (1-q)F \end{aligned}\right\} \text{Stripping section}$$



Assuming equimolar flow

$$L_n = L'_{f+1} - qF$$

$$\therefore L = L' - qF \quad \dots (13)$$

Underwood's Equations - Derivation

By rearranging Eq. 12 and Eq. 13, Underwood's Eq. 14 is obtained.

$$\sum_i \frac{\alpha_{1i} F x_{iF}}{k-\alpha_{1i}} = L - L' = -qF$$

$$\therefore \sum_i \frac{\alpha_{1i} x_{iF}}{k-\alpha_{1i}} = -q \qquad \left(\alpha_{1Lk} \le k \le \alpha_{1Hk}\right) \quad \ldots \text{ (14)}$$

If *k* is found by Eq. 14, the minimum reflux ratio can be obtained by Eq. 15.

$$\sum_i \frac{\alpha_{1i} D x_{iD}}{k-\alpha_{1i}} = L_{\min}$$

$$\therefore \sum_i \frac{\alpha_{1i} x_{iD}}{k-\alpha_{1i}} = \frac{L_{\min}}{D} = R_{\min} \quad \ldots \text{ (15)}$$

α_{1Lk} : Light key component
α_{1Hk} : Heavy key component

Underwoodの式 – 導出

By rearranging Eq. 11 and Eq. 12, Underwood's Eq. 13 is obtained.

$$\sum_i \frac{\alpha_{1i} F x_{iF}}{k-\alpha_{1i}} = L - L' = -qF$$

$$\sum_i \frac{\alpha_{1i} x_{iF}}{k-\alpha_{1i}} = -q \quad \ldots \text{ (13)}$$

$$\sum_i \frac{\alpha_{1i} x_{iF}}{k-\alpha_{1i}} = \frac{\alpha_{11} x_{1F}}{k-\alpha_{11}} + \frac{\alpha_{12} x_{2F}}{k-\alpha_{12}} + \cdots + \frac{\alpha_{1v} x_{vF}}{k-\alpha_{1v}}$$

Expansion example

If *k* is obtained by Eq. 13, the minimum reflux ratio can be obtained by Eq. 14

$$\sum_i \frac{\alpha_{1i} D x_{iD}}{k-\alpha_{1i}} = L_{\min}$$

$$\sum_i \frac{\alpha_{1i} D x_{iD}}{k-\alpha_{1i}} = \frac{L_{\min}}{D} = R_{\min} \quad \ldots \text{ (14)}$$

Underwood’s Equations - Application Example

Consider an example where the Underwood Equations are applied to a system of four components A, B, C, and D.

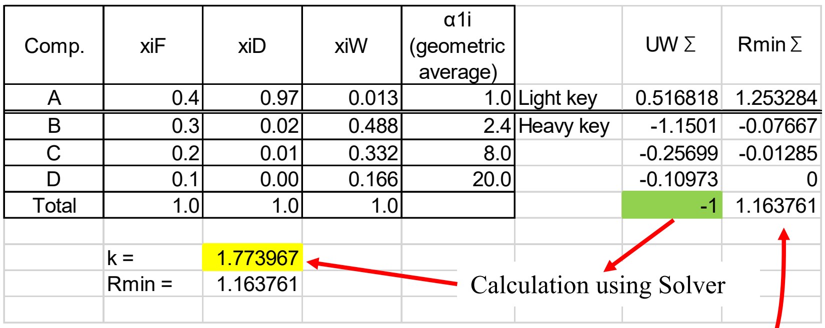
The feed compositions, top compositions, and relative volatilities are given in the following table. The purpose is to recover component A as the overhead product with a high purity.

The feed is a liquid at its boiling point ($q = 1$).

For the relative volatilities, geometric average values are used with respect to the top and bottom column temperatures.

Comp.	x_{iF}	x_{iD}	x_{iW}	α_{1i} (geometric average)
A	0.4	0.97	0.013	1.0
B	0.3	0.02	0.488	2.4
C	0.2	0.01	0.332	8.0
D	0.1	0.00	0.166	20.0
Total	1.0	1.0	1.0	

Underwood’s Equations - Application Example



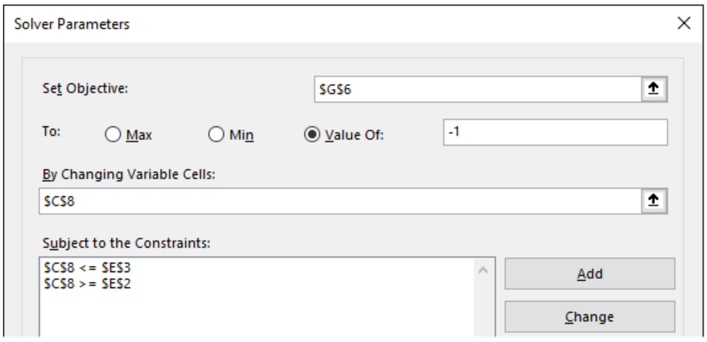
Comp.	xiF	xiD	xiW	α1i (geometric average)		UW Σ	Rmin Σ
A	0.4	0.97	0.013	1.0	Light key	0.516818	1.253284
B	0.3	0.02	0.488	2.4	Heavy key	-1.1501	-0.07667
C	0.2	0.01	0.332	8.0		-0.25699	-0.01285
D	0.1	0.00	0.166	20.0		-0.10973	0
Total	1.0	1.0	1.0			-1	1.163761
	k =	1.773967					
	Rmin =	1.163761					

Calculation using Solver

$$\sum_i \frac{\alpha_{1i}x_{iF}}{k-\alpha_{1i}} = \frac{\alpha_{11}x_{1F}}{k-\alpha_{11}} + \frac{\alpha_{12}x_{2F}}{k-\alpha_{12}} + \frac{\alpha_{13}x_{3F}}{k-\alpha_{13}} + \frac{\alpha_{14}x_{4F}}{k-\alpha_{14}} = -1$$

$$R_{\min} = \sum_i \frac{\alpha_{1i}x_{iD}}{k-\alpha_{1i}} = \frac{\alpha_{11}x_{1D}}{k-\alpha_{11}} + \frac{\alpha_{12}x_{2D}}{k-\alpha_{12}} + \frac{\alpha_{13}x_{3D}}{k-\alpha_{13}} + \frac{\alpha_{14}x_{4D}}{k-\alpha_{14}}$$

Solver settings



Solver Parameters

Set Objective: G6

To: ○ Max ○ Min ● Value Of: -1

By Changing Variable Cells: C8

Subject to the Constraints:
C8 <= E3
C8 >= E2

$k = 1.774$ and $R_{\min} = 1.16$ are obtained.
The theoretical number of stages can be determined by finding the optimal reflux ratio.

Reference: Optimal Reflux Ratio

When considering total costs, that is, the sum of fixed and operational costs , a minimum value of these costs can be found at a certain reflux ratio. *R* at this point is called the optimal reflux ratio and is usually expressed as *Ropt*.

Experience shows that the optimal reflux ratio *Ropt* is in the range of approximately 1.2 to 1.5 times the minimum reflux ratio *Rm*. However, in actual design, the reflux ratio is usually set slightly larger than *Ropt*. This is more convenient because it provides greater flexibility for the distillation equipment. Therefore, the following optimum reflux ratio is usually taken for design purposes.

Optimal reflux ratio: *Ropt* = 1.5 ~ 2.0×*Rm*

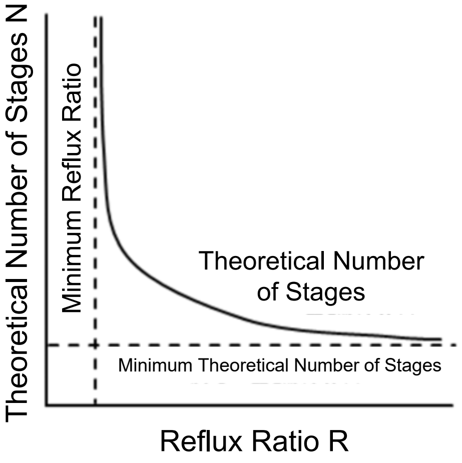
“Joryu no riron to keisan kogakutosho” *in Japanese*: Distillation Theory and Computation Engineering Books

Increasing the reflux ratio decreases the number of theoretical stages, but the vapor flow rate in the column increases, and the thermal load on the total condenser and the reboiler increases accordingly.

This is why there is an optimal value *Ropt* for the reflux ratio. Usually, the optimal reflux ratio (*Ropt*) falls within the following range.

(*Ropt* / *Rm* = 1.05 ~ 1.2)

“Kagaku Kougaku Binran Kaitei 6 Han” *in Japanese*: Chemical Engineering Handbook 6th ed.



Although it is necessary to comprehensively consider *Ropt* including costs and the like, in general, it is about 1.5 times *Rmin*.

Conclusion

- It has been seen that the minimum reflux ratio can be derived by the Underwood equations by using the concept of the pinch point where composition variations disappear.
- Since it is assumed that there is equimolar flow in the column and that the relative volatilities $\alpha_{i,j}$ are constant, this method applies only to ideal solution systems or systems for which relative volatilities are almost constant .
- A large number of components cannot be handled because calculation becomes complicated, but if the system for which relative volatilities are almost constant, the minimum reflux ratio for multicomponent distillation can be determined using the Underwood equations so that the approximate number of theoretical stages can be obtained.

Before performing rigorous calculations such as a simulation, it is important as well as effective to approximate the system by way of simple calculations.