Underwood's equations: derivation

Multicomponent distillation column design

The method is applied to all the i-components of a distillation, under the column's condition of minimum reflux. For a binary system, such a condition is represented in the composition diagram here below. A pinch point is present at stage j.



Figure 1: Pinch point condition for a binary system

For a multicomponent distillation, of course, the here above diagram can not be drawn. But the analytical condition for the pinch point can be written in any case.

Step 1

• Pinch point condition at stage j: the point representing the concentrations at stage j stays in the same time on the equilibrium curve and on the working line ⇒ the equilibrium and the working line compositions coincide. Please, refer to figure (2).

$$x_{j-1} = x_j = x_{j+1} \tag{1}$$

$$y_{j+1} = y_j = y_{j-1} \tag{2}$$

Step 2

• Mass balance around the red envelope in the rectification section as shown in figure (2) Mass balance for all the i components:

$$V_{\min} \cdot y_{j+1,i} = L_{\min} \cdot x_{j,i} + D \cdot x_{D,i} \tag{3}$$



Figure 2: Rectification section of column

Step 3

• Equilibrium condition for component i at stage (j+1):

$$y_{j+1,i} = k_i \cdot x_{j+1,i} \tag{4}$$

and because of the pinch condition it is also:

$$y_{j+1,i} = k_i \cdot x_{j,i} \tag{5}$$

where the distribution coefficient of the component i can be expressed through its constant of relative volatility α referred to a component r, which most often is the heavy key component (HK):

$$k_i = \alpha_{i,r} \cdot k_r \tag{6}$$

Step 4

• Substituting eqs. (5) and (6) in eq. (3) and rearranging:

$$\sum V_{min} \cdot y_{j+1,i} = \frac{\sum D \cdot x_{D,i}}{1 - \frac{L_{min}}{V_{min} \cdot \alpha_{i,r} \cdot k_r}}$$
(7)

which is convenient to write as follows:

$$V_{min} = D \cdot \sum \frac{\alpha_{i,r} \cdot x_{D,i}}{\alpha_{i,r} - \frac{L_{min}}{V_{min} \cdot k_r}}$$
(8)

In the same way for the stripping section a similar expression can be derived:

$$-V'_{min} = B \cdot \sum \frac{\alpha'_{i,r} \cdot x_{B,i}}{\alpha'_{i,r} - \frac{L'_{min}}{V'_{min\cdot k'}}}$$
(9)

Step 5

• Under the assumptions of CMO and of the constant of relative volatility (CRV) constance along the column:

$$\alpha_{i,r} = \alpha_{i,r}' \tag{10}$$

it can be proved that:

$$\phi = \frac{L_{min}}{V_{min} \cdot k_r} = \frac{L'_{min}}{V'_{min} \cdot k'_r} = \phi' \tag{11}$$

The term ϕ (or ϕ') has the dimension of a constant of relative volatility.

Step 6

• Underwood II: final expression.

Substituting eq. (12) in eq. (8), the final expression of the second Underwood equation is obtained:

$$V_{min} = D \cdot \sum \frac{\alpha_{i,r} \cdot x_{D,i}}{\alpha_{i,r} - \phi}$$
(12)

Step 7

• Underwood I: final expression

Subtracting eqs. (8) and (9) term by term and substituting the expression of eq. (12), yields:

$$V_{min} - V'_{min} = \sum \frac{\alpha_{i,r} \cdot (Dx_{D,i} + Bx_{B,i})}{\alpha_{i,r} - \phi}$$
(13)

and remembering that from a balance around the feed stage, it is valid the following expression:

$$V_{min} - V'_{min} = F(1 - q)$$
(14)

and from the overall mass balance it follows:

$$Dx_{D,i} + Bx_{B,i} = Fz_{F,i}$$
(15)

Substituting eqs. (15) and (16) in (14), the final expression of the **first Underwood equa**tion is obtained:

$$1 - q = \sum \frac{\alpha_{i,r} \cdot z_{F,i}}{\alpha_{i,r} - \phi} \tag{16}$$

ϕ calculation

for the Underwood's equations

Eq. (17) is a function of ϕ :

$$1 - q = \sum \frac{\alpha_{i,r} \cdot z_{F,i}}{\alpha_{i,r} - \phi} = f(\phi)$$

$$\tag{17}$$

whose derivate is always positive, as follows:

$$\frac{df}{d\phi} = \sum \frac{\alpha_{i,r} \cdot z_{F,i}}{\left(\alpha_{i,r} - \phi\right)^2} > 0 \tag{18}$$

This function can be represented as follows (blue line):



Figure 3: function of ϕ

c solutions are possible. 1 is negative hence meaningless. Among the other c-1 solution meaningful, the solution is the value of ϕ staying **between the** α_{LK} and α_{LK} , when the key components are **adjacent** in the scale of volatility:

$$\alpha_{_{LK}} > \phi > \alpha_{_{HK}} \tag{19}$$