

## 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  $j$ .

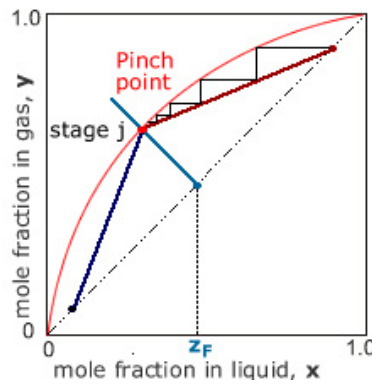


Figure 1: Pinch point condition for a binary system

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  $\implies$  the equilibrium and the working line compositions coincide. Please, refer to figure (2).

$$x_{j-1} = x_j = x_{j+1} \quad (1)$$

$$y_{j+1} = y_j = y_{j-1} \quad (2)$$

### Step 2

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

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

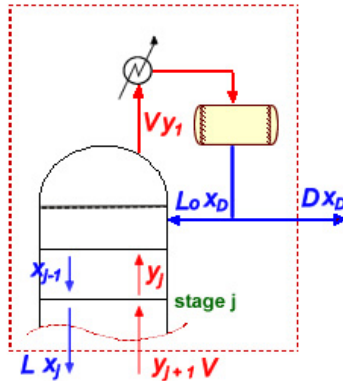


Figure 2: Rectification section of column

### Step 3

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

$$y_{j+1,i} = k_i \cdot x_{j+1,i} \quad (4)$$

and because of the pinch condition it is also:

$$y_{j+1,i} = k_i \cdot x_{j,i} \quad (5)$$

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

$$k_i = \alpha_{i,r} \cdot k_r \quad (6)$$

### Step 4

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

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

which is convenient to write as follows:

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

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

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

### Step 5

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

$$\alpha_{i,r} = \alpha'_{i,r} \quad (10)$$

it can be proved that:

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

The term  $\phi$  (or  $\phi'$ ) 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:

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

### Step 7

- Underwood I: final expression

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

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

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

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

and from the overall mass balance it follows:

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

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

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

### $\phi$ calculation for the Underwood's equations

Eq. (17) is a function of  $\phi$ :

$$1 - q = \sum \frac{\alpha_{i,r} \cdot z_{F,i}}{\alpha_{i,r} - \phi} = f(\phi) \quad (17)$$

whose derivate is always positive, as follows:

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

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

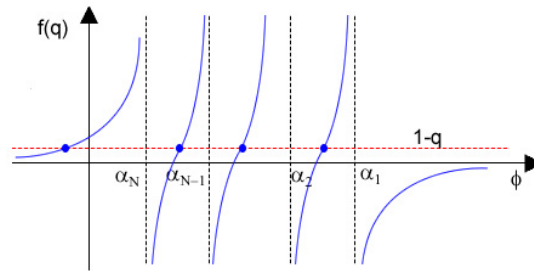


Figure 3: function of  $\phi$

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

$$\alpha_{LK} > \phi > \alpha_{HK} \quad (19)$$