Ideal systems

These systems are governed by Raoult's law and Dalton's law

$p_A = p_A^O x_A$ ……………. (Raoult's law) ….(1)

$P = p_A + p_B$ ……….…... (Dalton's law) ….(2)

Where

p_A = partial pressure of component A

p_A^O = vapor pressure of component A

x_A = mole fraction of component A in the liquid phase

P = total pressure

From equations 1 and 2 we can conclude that:

$$x_A = \frac{P - p_B^O}{p_A^O - p_B^O}$$

$$y_A = \frac{p_A^O x_A}{P}$$

Relative volatility

It is a measure of the differences in volatility between two components and hence their boiling points. It indicates how easy or difficult a particular separation will be.

If the relative volatility between two components equals one, separation by distillation is not possible. The larger the value of relative volatility above 1, the greater the degree of separability, i.e, the easier separation. Relative volatility is denoted by α.

Suppose that we have a binary mixture (A & B)

$$\alpha_A = \frac{p_A^O}{P}$$

$$\alpha_B = \frac{p_B^O}{P}$$

$$\alpha_{AB} = \frac{p_A^O / P}{p_B^O / P} = \frac{p_A^O}{p_B^O}$$

$$y_A = \frac{p_A^O x_A}{P}$$

$$p_A^O = \frac{y_A P}{x_A}$$

Similarly

$$p_B^O = \frac{y_B P}{x_B}$$

$$\alpha_{AB} = \frac{p_A^O}{p_B^O} = \frac{\frac{y_A P}{x_A}}{\frac{y_B P}{x_B}}$$

$$\alpha_{AB} = \frac{y_A / x_A}{y_B / x_B}$$

$$\alpha_{AB} = \frac{y_A / x_A}{(1 - y_A)/(1 - x_A)}$$

From which

$$y_A = \frac{\alpha_{AB} x_A}{1 + (\alpha_{AB} - 1) x_A}$$

Note:

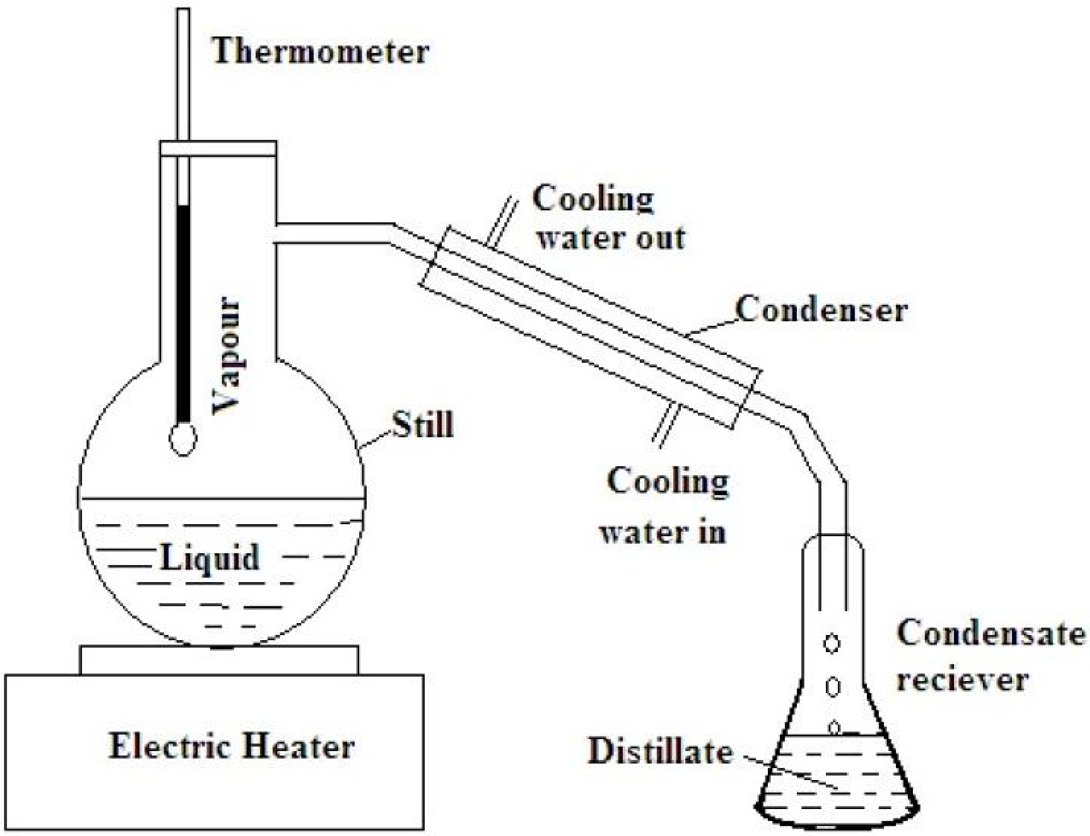
For non-ideal system:

$$y_A = \gamma_A p_A^O x_A$$

Differential distillation columns and their process calculation

In batch mode of operation, the feed is introduces batch-wise to the column, that is the column is charged with a batch, then the distillation process is carried out. When the desired task is achieved, a next batch of feed is introduced.

Consider a binary mixture of component A (more volatile component) and B (less volatile component). The system consists of a batch of liquid (fixed quantity) inside a container or vessel fitted with a heater and condenser to condense the vapor produced as shown in figure below:



Material balance

Initial amount of A in vessel = Amount left in vessel + amount vaporized

$x_A L = (x_A - dx_A)(L - dL) + y_A dL$

$x_A L = x_A L - x_A dL - L dx_A + dx_A dL + y_A dL$

Neglecting dxAdL

$$x_A dL = y_A dL - L dx_A$$

From which

$$\frac{dL}{L} = \frac{dx_A}{y_A - x_A}$$

$$\int_{L_1}^{L_2} \frac{dL}{L} = \int_{x_{A1}}^{x_{A2}} \frac{dx_A}{y_A - x_A}$$

$\ln \frac{L_1}{L_2} = \int_{x_{A2}}^{x_{A1}} \frac{dx_A}{y_A - x_A}$ Rayleigh equation

Where

L1 = initial amount of liquid batch

L2 = final amount of liquid batch (residue in the still)

xA1 = initial concentration (mole fraction) of the more volatile component in the liquid feed batch.

xA2 = final concentration (mole fraction) remained in the liquid feed batch.

yA = mole fraction of the more volatile component in the vapor phase.

Note:

Rayleigh equation could be solved analytically or graphically.

- By analytical solution:

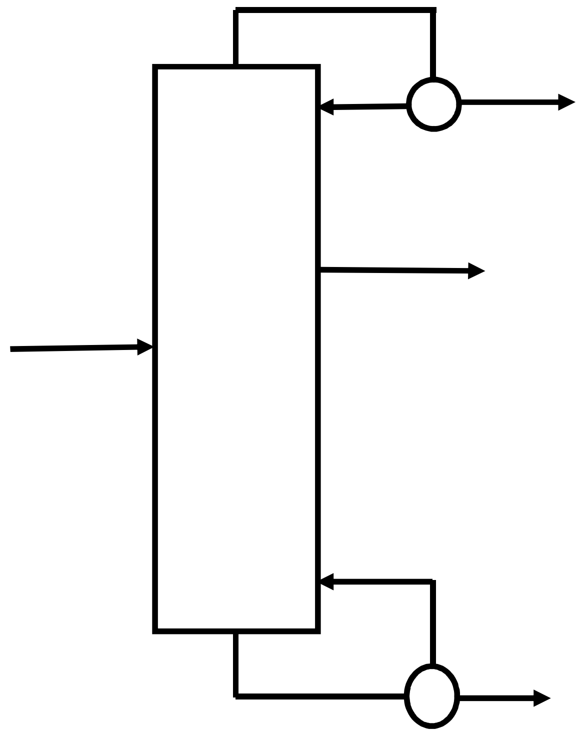
$$\ln \frac{L_1}{L_2} = \frac{1}{\alpha_{AB} - 1} [ln \frac{x_{A1}}{x_{A2}} - \alpha_{AB} ln \frac{1 - x_{A1}}{1 - X_{A2}}]$$

By graphical method:

$$plot\ \frac{1}{y_A - x_A}\ versus\ x_A\ and\ find\ the\ area\ under\ the\ curve.$$

Binary multiple side streams (McCabe-Thiele method)

Similar to multiple feeds, multiple mass balance envelopes could be used. Consider the figure below:



The column in this case consists of three parts (three sections). As shown in this figure, section 1 will start from the column top and will not include the side stream, so, the operating line for this section will be the rectifying section operating line

$$y_n = \frac{L_1}{V_1} x_{n+1} + \frac{D}{V_1} x_d$$

For section 2, the envelope will include the side stream, and the material balance for this section will be:

In = Out

$$V_2 y_n = L_2 x_{n+1} + D x_d + S x_s$$

$$y_n = \frac{L_2}{V_2} x_{n+1} + \frac{D x_d + S x_s}{V_2}$$

Where

S = flow rate of side stream

x_s = concentration of the side stream.

Now, material balance for the third section will give the operating line for striping section:

$$y_m = \frac{L_3}{V_3} x_{m+1} + \frac{W}{V_3} x_w$$

Example:

A mixture of 50 % n-hexane and 50 % n-heptane is subjected to continuous fractionation in a tray column at 1 atm total pressure at feed rate of 100 kmol/h. a liquid side stream of 70 % n-hexane is to be withdrawn at a rate of 20 kmol/h. the top product contains 90 % n-hexane and the residue contains 5 % n-hexane.

The feed is saturated liquid. The reflux is a saturated liquid and the reflux ratio of 2.5 is used. The relative volatility of n-hexane in the mixture is 2.36.

Find out the number of ideal trays required foe the given separation and identify the tray from which the side stream should be withdrawn.

Solution:

Section 1:

$$y_n = \frac{L_1}{V_1}x_{n+1} + \frac{D}{V_1}x_d$$

$$R = \frac{L_1}{D}$$

$$V_1 = L_1 + D$$

Overall material balance

F = D + W + S

100 = D + W + S

$$Fx_f = Dx_d + Wx_w + Sx_s$$

(100)(0.5) = D(0.9) + W(0.05) (20)(0.7)

From which

D = 35.56 kmol/h

W = 44.44 kmol/h

V1 = (R+1)*D = (2.5+1)(35.56) = 124.46 kmol/h

L1 = R*D = (2.5)(35.56) = 88.9 kmol/h

So, for section 1:

$$y_n = \frac{88.9}{124.46}x_{n+1} + \frac{35.56}{124.46}$$

$$y_n = 0.714x_{n+1} + 0.285$$

For section (2)

Material balance on this section:

In = Out

$$V_2y_n = L_2x_{n+1} + Dx_d + Sx_s$$

$$y_n = \frac{L_2}{V_2} x_{n+1} + \frac{Dx_d + Sx_s}{V_2}$$

V2 = V1 = 124.46 kmol/h

L2 = L1 – S = 88.9 – 20 = 68.9 kmol/h

$$y_n = \frac{68.9}{124.46} x_{n+1} + \frac{(35.56)(0.9) + (20)(0.7)}{124.46}$$

$$y_n = 0.553x_{n+1} + 0.369$$

q value

The side stream is saturated liquid

$$q = \frac{\lambda}{\lambda} = 1$$

$$slope = \frac{-q}{1-q} = \frac{-1}{1-1} = \infty$$

$$\theta = 90^O$$

Similarly, the feed is saturated liquid

$$q = \frac{\lambda}{\lambda} = 1$$

$$slope = \frac{-q}{1-q} = \frac{-1}{1-1} = \infty$$

$$\theta = 90^O$$

From the graph, we get:

Total number of plates = 8

Feed plate = 4

Side stream plate = 2

Multicomponent distillation

Number of distillation towers

- **Binary system**

One tower could be used to separate two components into relatively pure components.

- **Multicomponent system**

n-1 fractionators are required for the separation of n components. For example, for 3 components, the number of fractionators will be (3-1 = 2 fractionators)

Equilibrium in multicomponent system

Experimental vapor-liquid equilibrium data are not known in most multicomponent systems, so, the data could be computed from available equations or relations. Ideal behavior may be assumed so that Raoult's law is applicable:

$$p_i = x_i * p_i^O$$

where

$p_i = partial\ pressure\ of\ component\ i\ in\ vapor\ phse$

$p_i^O = vapor\ pressure\ of\ component\ i$

$x_i = mole\ fraction\ of\ component\ i\ in\ the\ liquid\ phase$

And also:

$$P = \sum_{i=1}^{i=n} p_i$$

Where

P = total pressure

Also remember that:

$$\alpha_{ij} = \frac{\alpha_i}{\alpha_j} = \frac{p_i^O}{p_j^O}$$

And

$$y_j = \frac{\alpha_{jk} x_j}{\sum(\alpha x)_i}$$

Where k is a reference component

For example, if we have four components A, B, C, and D, and the reference component is D, then:

$$y_A = \frac{\alpha_{AD}x_A}{\alpha_{AD}x_A + \alpha_{BD}x_B + \alpha_{CD}x_C + \alpha_{DD}x_D}$$

$$y_B = \frac{\alpha_{BD}x_B}{\alpha_{AD}x_A + \alpha_{BD}x_B + \alpha_{CD}x_C + \alpha_{DD}x_D}$$

$$y_C = \frac{\alpha_{CD}x_C}{\alpha_{AD}x_A + \alpha_{BD}x_B + \alpha_{CD}x_C + \alpha_{DD}x_D}$$

$$y_D = \frac{\alpha_{DD}x_D}{\alpha_{AD}x_A + \alpha_{BD}x_B + \alpha_{CD}x_C + \alpha_{DD}x_D}$$

Light and heavy key components:

If the fractionation of multicomponent mixtures, the aim will be the separation of two components. These two components are called key components.

Consider that we have four components mixture A-B-C-D in which (A) is the most volatile and D is the least volatile and the other components are arranged according to their volatilities as shown below:

A ………….. most volatile

B

C

D …………… least volatile

The first thing that we have to do is to decide the two components those we want to separate. These two components are called (key components). The key components (both key components) should appear in both top and bottom products.

Note:

The light key component (LK) appears mostly in the top product, while the heavy key component (HK) appears mostly in the bottom product.

Calculation of the number of plates required for a given separation

For the case of multicomponent system, use the following steps:

1- Construct the operating line's equation for each component in each section in the column.
2- The equilibrium relation for this case will be:

$$y_j = \frac{\alpha_{jk} x_j}{\sum(\alpha x)_i} \quad \text{…………….} \ (1)$$

Where

K = reference component

α_{jk} = relative volatility of component j with respect to the reference component k.

3- Calculate the number of plates step by step by using (Lewis and Matheson) method which is based on Lewis Sorel method.
4- Starting from the bottom, calculate y_O for each component by substitute the values of x_W in equation 1

Example:

A mixture of ortho, meta, para-mononitrotoluenes containing 60, 4, 36 mole percent respectively of the three isomers is to be continuously distilled to give a top products of 98% ortho, 0.6% meta and 1.4% para, and the bottom is 12.5% ortho. The mixture that to be distilled at a temperature of 410 K is saturated liquid and the operating pressure is 6 kN/m^2. If a reflux ratio of 5 is used, how many ideal plates will be required and what will be the approximate compositions of the product streams?

The volatility of ortho to para isomer may be taken as 1.7 and of meta as 1.16 over the temperature range of 380 to 415 K. the feed flow rate is 100 kmol/h.

Example:

A liquid mixture of benzene and toluene is being distilled in a fractionating column at 101.3 kpa pressure. The feed of 100 kmol/h is liquid and it contains 45% benzene (A) and 55% toluene (B) and enters at 327.6 K. the distillate containing 95% benzene and 5% toluene (B), and bottom contains 10% benzene and 90% toluene. The amount of liquid fed back to the column at the top is 4 time the distillate product. The average heat capacity of the feed is 159 kJ/kg.mol.k and the average latent heat is 32099 kJ/kmol and the bubble temperature of feed is 366.7 K. calculate:

1- D and W
2- Number of theoretical plate.

The equilibrium data for this this system is given in the following table:

x_A	1	0.78	0.58	0.45	0.258	0.13	0
y_A	1	0.9	0.777	0.657	0.456	0.261	0

Solution:

Overall material balance:

In = Out

F = D + W

100 = D + W ………….. (1)

Fxf = Dxd + Wxw

(100)(0.45) = D(0.95) + W(0.1) ………(2)

From equations 1 & 2

D = 41.2 kmol / h

W = 58.8 kmol/h

Determination of ROL:

$$slope = \frac{R}{R+1} \ \& \ intercept = \frac{x_d}{R+1}$$

$$slope = \frac{4}{4+1} = 0.8$$

$$intercept = \frac{0.95}{4 + 1} = 0.19$$

Determination of feed conditions

$$q = \frac{C_p\left(T_b - T_f\right) + \lambda}{\lambda} = \frac{159(366.7 - 327.6) + 32099}{32099} = 1.193$$

q = 1.193

$$slope = \frac{-q}{1 + q} = \frac{-1.193}{1 - 1.193} = 6.18$$

$$\theta = 80.8^{O}$$

From the graph, we can find that:

Total number of theoretical stages = 8 plates.