Chapter 5: Part 1

Simplified VLE Calculations

When K_i is independent of concentration

"Bubble T" problem (from lecture 4)

Specify: $x_1, x_2 \ldots P$

calculate: $y_1, y_2 \ldots T$

$\hat{\phi}_i$ = fugacity coefficient
γ_i = activity coefficient of i

Method 1:

Assume $\hat{\phi}_i = \gamma_i = 1$

and $K_i = \dfrac{P_{i,sat}}{P} = \dfrac{\exp\left(A_i - \dfrac{B_i}{T+C_i}\right)}{P}$

Antoine equation

We know $\sum y_i = 1$ or $1 - \sum y_i = 0$

Substituting $y_i = K_i x_i$

$$0 = 1 - \sum_i K_i x_i = 1 - \sum_i \frac{\exp\left(A_i - \dfrac{B_i}{T+C_i}\right) x_i}{P}$$

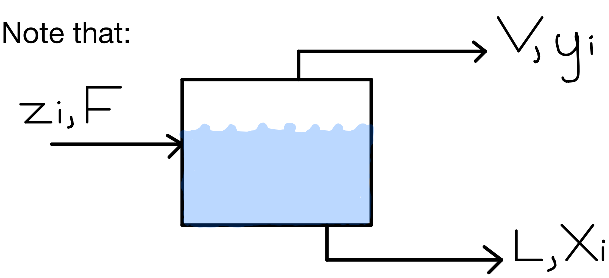
- Solve for T, then determine K_i, then y_i

Method 2:

Alternatively, use De Priester chart, which assumes $\phi_i = \gamma_i$ =constant but not unity

Flash concentration with T and P specified and K_i independent of composition

Note that:



1. $x_i L + y_i V = z_i F$
2. $L + V = F$
3. $y_i = K_i x_i$

Combine 1,2 and 3 to eliminate xi and L:

$$y_i = \frac{K_i z_i}{(K_i - 1)\dfrac{V}{F} + 1}$$

Combine 1,2 and 3 to eliminate yi and L:

$$x_i = \frac{z_i}{(K_i - 1)\dfrac{V}{F} + 1}$$

K_i is a function of T and P but assume that it's not a function of composition

"Best" check function- residual solved by trial and error

$$\underbrace{f\left(\frac{V}{F}, T, P\right)}_{\text{If 2 are known, you can solve for the third}} = \sum X_i - \sum y_i = \sum \frac{z_i(K_i-1)}{(K_i-1)\frac{V}{F}+1} = 0$$

Rachford-Rice equation

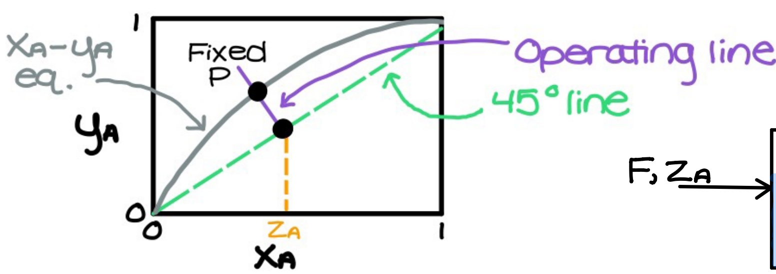
For example, if T and P are given, then K_i is known and $\left(\frac{V}{F}\right)$ can be determined numerically.

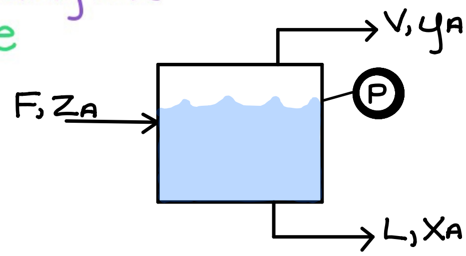
$$f\left(\frac{V}{F}\right) = 0 \implies \left(\frac{V}{F}\right)_{i+1} = \left(\frac{V}{F}\right)_i - \frac{f\left(\left(\frac{V}{F}\right)_i\right)}{f'\left(\left(\frac{V}{F}\right)_i\right)}$$

Then back-substitute to determine x_i and y_i.

Graphical solution of a binary flash process on a y_A - x_A diagram:

Fix P and L/V for a binary (A+B) mixture





Material balance:

$$Fz_A = y_A V + x_A L$$

Solve for y_A: $$y_A = \underbrace{\frac{F}{V} z_A}_{\text{intercept}} - \underbrace{\frac{L}{V}}_{\text{slope}} x_A$$ "operating" line

The above equation gives possible y_A and x_A values for specified z_A and L/V.

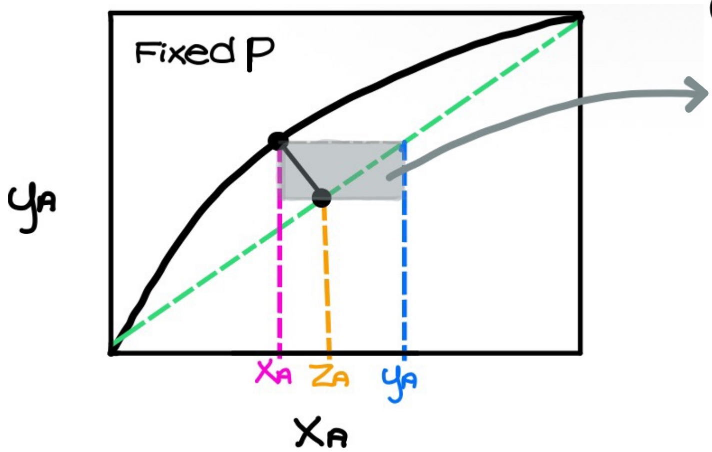
Intersection of operating line with 45° line:

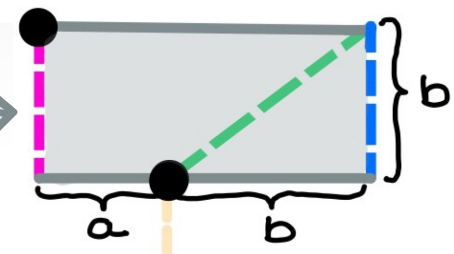
Since $y_A = x_A$ on the 45° line, we get:

$$x_A = \frac{F}{V} z_A - \frac{L}{V} x_A \implies z_A = x_A = y_A$$

This is also an example of the **lever rule** since the first equation can be written as

$$(V+L)z_A = y_A V + x_A L \implies \frac{z_A - y_A}{z_A - x_A} = \frac{-L}{V}$$

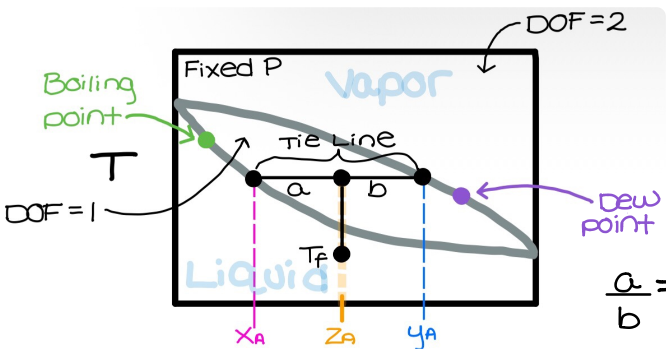


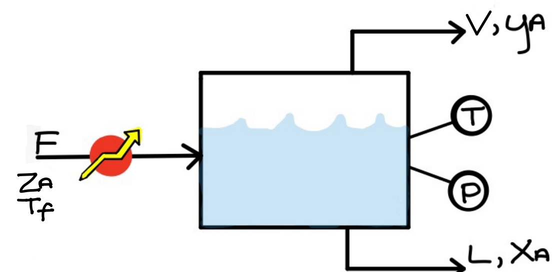


$$\frac{b}{a} = \frac{L}{V}$$

Lever Rule

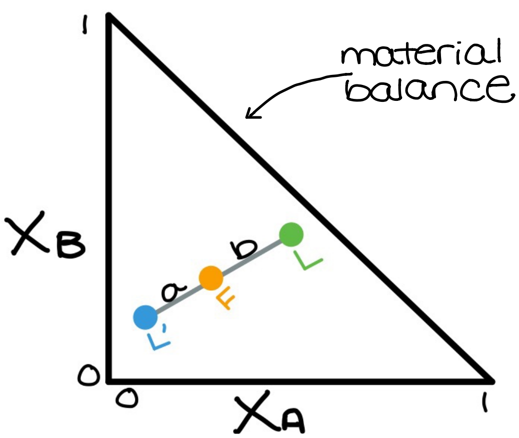
Another example: T-x_A-y_A diagram

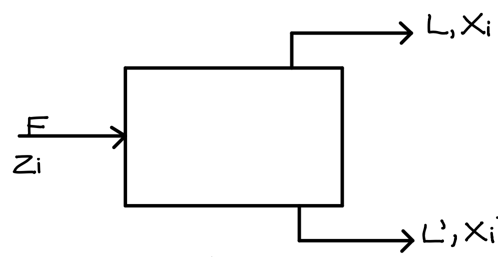




$$\frac{a}{b} = \frac{V}{L}$$

Three component system: 3 independent material balances (A,B,or C)

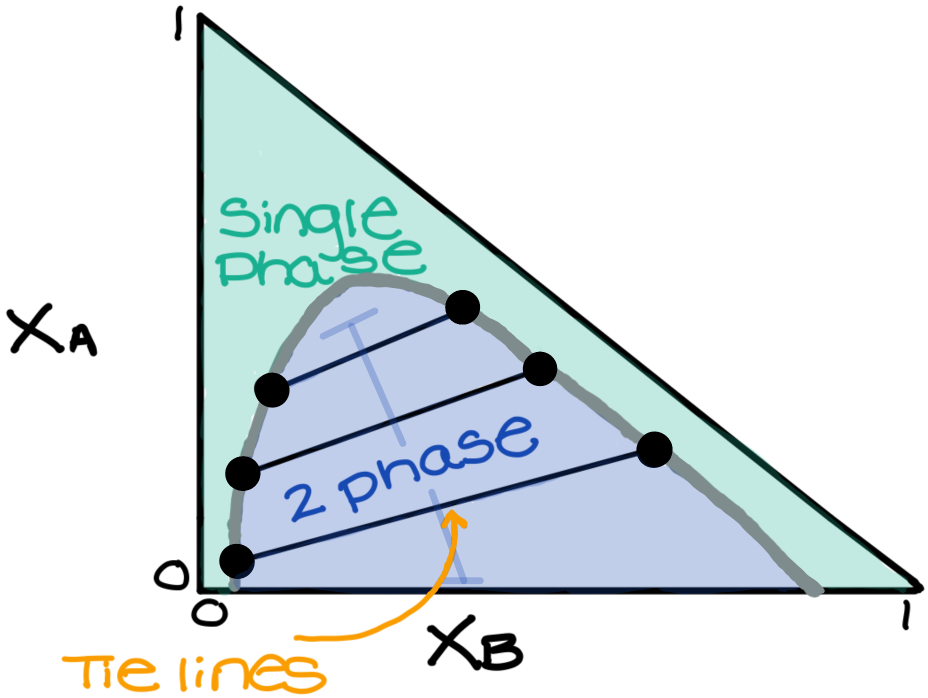




$$\frac{a}{b} = \frac{L}{L'}$$

$$x_c = 1 - x_A - x_B$$

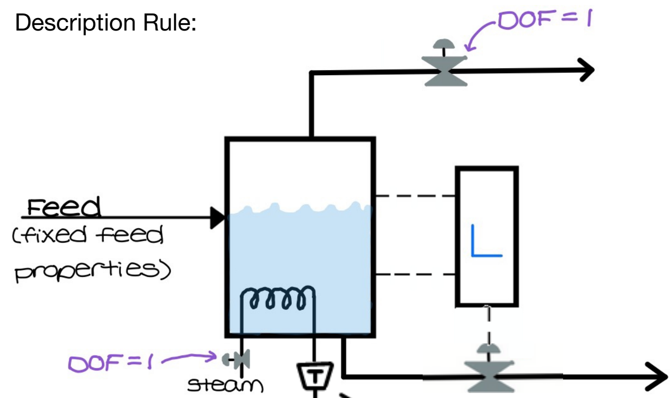
Phase equilibrium



Flash Calculations:

General approach when K_i is a function of composition

Description Rule:

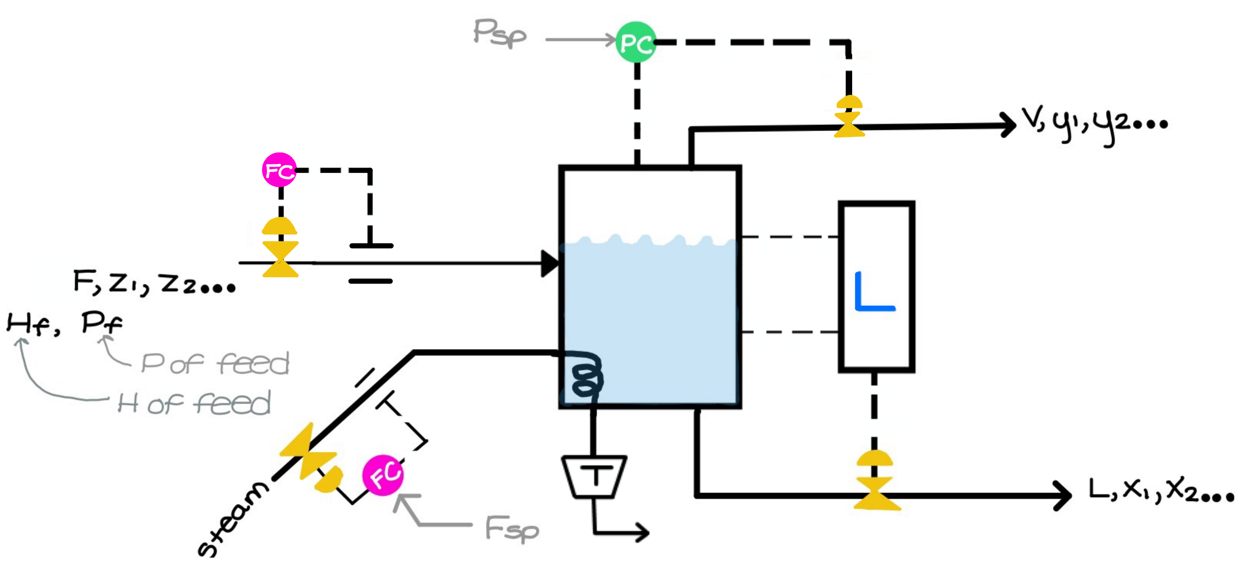


2 values = 2 DOF

Total DOF=2 if feed properties are fixed

See Chapter 5 (part 2) for a discussion of the degree of freedom (DOF) analysis

Specifying **<u>product enthalpy</u>** **and** **<u>product pressure</u>** is equivalent to using the following control system which uses up to the available DOF



For 5 components we have the following:

<u>Specified</u>: $z_1, z_2, z_3, z_4, z_5, F, P_F, H_F, Q, P$

<u>Calculate</u>: $x_1, x_2, x_3, x_4, x_5, y_1, y_2, y_3, y_4, y_5, \frac{V}{F}, T$ ($\frac{L}{F}$ not treated as independent since $\frac{L}{F} + \frac{V}{F} = 1$)

a.k.a. determine or unknown

12 variables means that we need 12 equations

Equations:

Phase Equilibrium:

$$y_1 - \frac{x_1 \gamma_1 \phi_{1,sat} P_{1,sat}}{P \hat{\phi}_1} = 0 \quad (1)$$

$$y_2 - \frac{x_2 \gamma_2 \phi_{2,sat} P_{2,sat}}{P \hat{\phi}_2} = 0 \quad (2)$$

$$y_3 - \frac{x_3 \gamma_3 \phi_{3,sat} P_{3,sat}}{P \hat{\phi}_3} = 0 \quad (3)$$

$$y_4 - \frac{x_4 \gamma_4 \phi_{4,sat} P_{4,sat}}{P \hat{\phi}_4} = 0 \quad (4)$$

$$y_5 - \frac{x_5 \gamma_5 \phi_{5,sat} P_{5,sat}}{P \hat{\phi}_5} = 0 \quad (5)$$

Material Balances:

$$y_1\left(\frac{V}{F}\right) + x_1\left(1 - \frac{V}{F}\right) - z_1 = 0 \quad (6)$$

$$y_2\left(\frac{V}{F}\right) + x_2\left(1 - \frac{V}{F}\right) - z_2 = 0 \quad (7)$$

$$y_3\left(\frac{V}{F}\right) + x_3\left(1 - \frac{V}{F}\right) - z_3 = 0 \quad (8)$$

$$y_4\left(\frac{V}{F}\right) + x_4\left(1 - \frac{V}{F}\right) - z_4 = 0 \quad (9)$$

$$y_5\left(\frac{V}{F}\right) + x_5\left(1 - \frac{V}{F}\right) - z_5 = 0 \quad (10)$$

$$y_1 + y_2 + y_3 + y_4 + y_5 - 1 = 0 \quad (11)$$

$$H_f + \frac{Q}{F} = \frac{V}{F} H_V + \left(1 - \frac{V}{F}\right) h_L \quad (12)$$

For simplicity, assume that there are no heat of mixing effects so that, if enthalpy of pure liquid i is set = 0 at 298:

$$h_L = \sum x_i C_{pi,l} (T - 298)$$

$$H_V = \sum y_i \left(C_{pi,l} (T - 298) + \Delta H_{v,i}\right)$$

assume $C_{pi,l}$ is constant