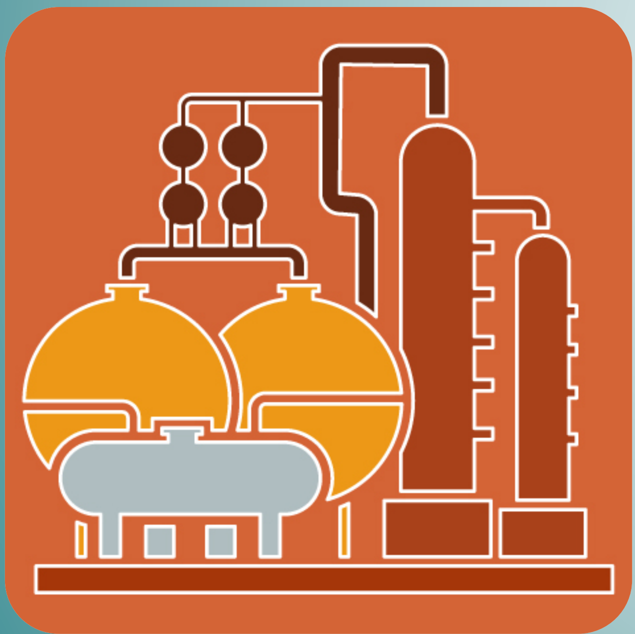
Chemical Process Design / Diseño de Procesos Químicos

Topic 4.7. Flash



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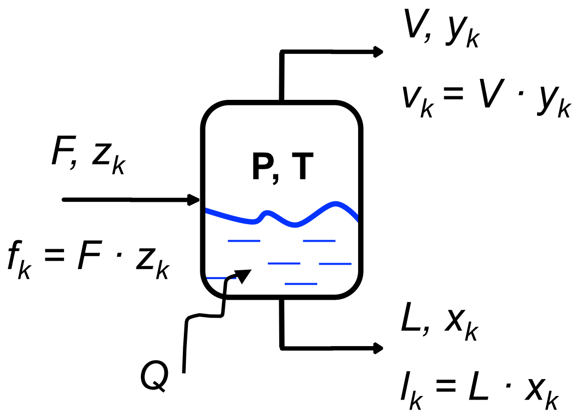
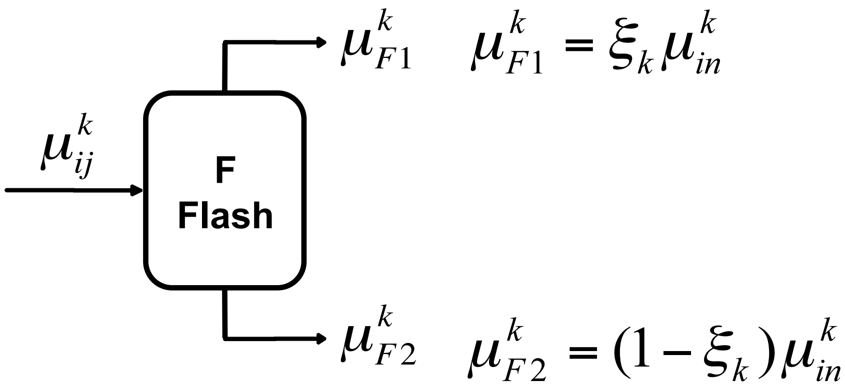
4.- Development of Linear Mass Balance (LMB) models

φ	fi
ξ	xi

4.3. Flash: Module used to build other separation modules, such as distillation or adsorption



Representation the flash as a Splitter.



Define:

a) "Split fraction component **k** in vapor" $\xi_k = \dfrac{v_k}{f_k}$

b) Key component (or the reference) $k = n$

c) Fraction of **F** as Vapor (Vaporization) $\varphi = \dfrac{V}{F}$

Variables that are usually specified ξ_n, φ, P, T, Q

What's important is to obtain the split fraction, but fulfilling the liquid-vapor equilibrium at flash operation conditions of T and P.

- Flash unit with feed stream defined has **2 degrees of freedom** → Thermodynamic subject.
- We **exclude the choice of Q** as variable to maintain the linear mass balance

→ **Decoupled Mass and Energy balances**.

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Φ φ fi

Consider the following cases:

- **Case 1.** Specification of ξ_n and **P** or **T**. **Fixed Recovery Flash**. “More used case”).
- **Case 2.** φ specified and **T** or **P**. **Fixed Vaporization Flash**.
- **Case 3. T** and **P** specified. **Isothermal Flash**.

Important → Phase Equilibrium

Vapor/liquid phase equilibrium $f_v^k = f_l^k$ for all components **k**.

$$\phi_k \cdot y_k \cdot P = \gamma_k \cdot x_k \cdot f_k^0 \quad \textbf{(Eq. 1)}$$

Where: ϕ_k Vapor fugacity coefficient.

γ_k Liquid activity coefficient.

f_k^0 Pure component fugacity.

To simplify: ideal behavior which leads to the following assumptions: $\phi_k = 1 \quad \gamma_k = 1 \quad f_k^0 = P_k^0$

Antoine equation for vapor pressure $LnP_k^0 = A_k - \dfrac{B_k}{T + C_k}$ Coefficients can be found in Reid *(et al.)*, 1987.

From Eq. 1 $y_k \cdot P = x_k \cdot P_k^0$ **Raoult Law**

We define the equilibrium constant $K_k = \dfrac{y_k}{x_k} = \dfrac{P_k^0}{P}$ **(Eq. 2)**

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Define a relative volatility: $\alpha_{k/n} = \frac{K_k}{K_n} = \frac{P_k^0}{P_n^0}$

If **k** is non volatile: $\alpha_{k/n} \cong 0$

If **k** is non condensable: $\alpha_{k/n} \cong \infty$

If you know **T**, you know **P⁰** with Antoine, and then you know: $\alpha_{k/n}$

Now, we redefine relative volatility as: $\alpha_{k/n} = \frac{K_k}{K_n} = \frac{y_k / x_k}{y_n / x_n} \frac{V/L}{V/L} = \frac{v_k / l_k}{v_n / l_n}$ **(Eq. 3)**

Reintroduce the split fraction and define: $v_k = \xi_k f_k$ **(Eq. 4)** $l_k = (1-\xi_k) f_k$ **(Eq. 5)**

Substitutes in **Eq. 3**: $\alpha_{k/n} = \frac{\xi_k /(1-\xi_k)}{\xi_n /(1-\xi_n)}$

We can express ξ_k in function ξ_n of $\alpha_{k/n}$, obtaining: $\xi_k = \left[\frac{\alpha_{k/n}\, \xi_n}{1 + (\alpha_{k/n} - 1)\, \xi_n} \right]$ For all k ≠ n.

For limiting cases:

- If **k** is non volatile (heavy component, like Toluene): $\alpha_{k/n} \to 0 \longrightarrow \xi_k \to 0$
- If **k** is non condensable (Volatile component, like $\mathbf{H_2}$): $\alpha_{k/n} \to \infty \longrightarrow \xi_k \to 1$

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How can you calculate **P** (or **T**) from the solved mass balance? or How can you check if the **T** (or **P**) guess is correct?

We consider equilibrium using the **Bubble Point Equation or Dew Point Equation**.

- At bubble point (for the saturated liquid effluent stream):

$$\sum y_i = \sum K_i x_i = 1 \quad \text{as,} \quad K_k = \frac{y_k}{x_k} = \frac{P_k^0}{P} \rightarrow \sum (P_i^0 / P) x_i \rightarrow P = \sum P_i^0(T) x_i$$

Bubble Point Equation, where we need all expression of **$P^0(T)$** for each component **i**. For this reason we obtain the Bubble Point Equation in terms of relative volatility $\bar{\alpha}$:

$$\bar{\alpha} = \sum \alpha_{i/n} x_i = \sum (K_i / K_n) x_i = 1 / K_n$$

Substituting in **Eq. 2**: $\frac{P_k^0}{P} = K_k = \frac{\alpha_{k/n}}{\bar{\alpha}}$

1. For **T** fixed and **P** unknown → $P = \frac{\bar{\alpha}}{\alpha_{k/n}} P_k^0(T)$

2. For **P** fixed and **T** unknown → $P_k^0(T) = \frac{\alpha_{k/n}}{\bar{\alpha}} P$

Using the Bubble Point Equation, to reduce approximation errors, choose **k** to be the most abundant component in liquid phase.

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Algorithms for the three cases:

- **Case 1.** ξ_n **and P (or T) Fixed. Fixed Recovery Flash. "More used case".**

1. Choose key component **n**, specified ξ_n and **P** (or **T**), guess **T** (or **P**).

2. Calculate $\mathbf{K_k}$, $\alpha_{k/n}$ at specified **T**.

3. Evaluate $\xi_k = \left[\dfrac{\alpha_{k/n}\,\xi_n}{1+(\alpha_{k/n}-1)\,\xi_n} \right]$ for each component **k**.

4. Solve equations mass balances for all **k**:

$$v_k = \xi_k f_k \qquad y_k = v_k / \sum v_i$$

$$l_k = (1-\xi_k) f_k \qquad x_k = l_k / \sum l_i$$

5. For **T** specified, calculate: $P = \dfrac{\bar{\alpha}}{\alpha_{k/n}} P_k^0(T)$

Compare this P from the mass balance with initial P from my guess is Step 1.

For **P** specified, calculate: $P_k^0(T) = \dfrac{\alpha_{k/n}}{\bar{\alpha}} P$

Compare this T from the mass balance with initial T from my guess in Step 1.

If **T** (or **P**) calculated is different to **T** (or **P**) guesses, return to **Step 2** with new **T** (or **P**) guess .

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Algorithms for the three cases:

- **Case 2.** φ **and P (or T) Fixed. Fixed Vaporization Flash.**

1. Choose key component **n**, specified $\varphi = V/F$ and **P** or **T**.

2. Guess ξ_n , calculate $\mathbf{K_k}$, and

3. Evaluate $\xi_k = \left[\dfrac{\alpha_{k/n}\, \xi_n}{1 + (\alpha_{k/n} - 1)\, \xi_n} \right]$ for each component **k**.

4. Solve equations mass balances for all **k**:

$$v_k = \xi_k f_k \qquad y_k = v_k / \sum v_i$$

$$l_k = (1 - \xi_k) f_k \qquad x_k = l_k / \sum l_i$$

5. If **V/F** ≈ φ go to **Step 6**, otherwise go to **Step 2** and re-guess ξ_n

6. Calculate **P** (or **T**) from the bubble point equation to calculate **P** or **T**.

$$P = \frac{\bar{\alpha}}{\alpha_{k/n}} P_k^0(T) \qquad P_k^0(T) = \frac{\alpha_{k/n}}{\bar{\alpha}} P$$

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Algorithms for the three cases:

- **Case 3. P and T Fixed. Isothermal Flash. Typically in the reactor downstream.**

1. Choose key component **n**, and guess ξ_n .

Follow **Step 2** ($\alpha_{k/n}$) and **Step 4** ($\mathbf{v_k}$, $\mathbf{l_k}$, $\bar{\alpha}$) of algorithm **Case 1**.

5. If the bubble point equation is satisfied $\bar{\alpha} = P\alpha_{k/n} / P_k^0 \longrightarrow$ Stop.

Otherwise re-guess ξ_n and start again.