Mass transfer

Lecture 16: *Multicomponent distillation*

Jamin Koo

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Learning objectives

- **Understand how equilibrium constraints and material balance equations are used in analyzing multicomponent distillation.**

- **Use computational methods to estimate number of plates, reflux ratio, and other parameters for designing a fractionating column.**

Today's outline

- **Phase equilibria**
  - ✓ Distribution coefficient
  - ✓ Bubble point (bp), and due point (dp) calculation

- **Flash distillation**

- **Fractionating column**
  - Minimum number of plates N
  - Minimum reflux ratio R
  - Material balance

22.1 Distribution coefficients

- **Distribution coefficient (or K factor):**

$$K_i \equiv y_{i,e}/x_{i,e}$$

where $y_{i,e}$ and $x_{i,e}$ are the liquid and gas mole fraction of component *i* in equilibrium with others.

✓ For ideal mixtures,

$$p_i = x_i \, P_i'$$

$$y_i = \frac{p_i}{P}$$

$$K_i = \frac{x_i \, P_i'}{P \, x_i} = \frac{P_i'}{P}$$

where p_i and P_i' are partial pressure and vapor pressure of component *i* (difference between the two? Temp. dependence)

✓ Applicability of Raoult's law?

✓ The eqn for K factor is not applicable at high pressures (> 20 atm) compressibility effects.

22.1 Bp & dp estimation

- **Bubble point and due point of ideal mixtures (*N* components) can be calculated by the following procedure:**

  Why do we need this information?

  (1) Assume a temperature and total pressure (x_i are provided)

  (2) Obtain values of K_i for each component using literature.

  (3) If the assumed temperature is indeed the bubble point (why not dp),

  $$\sum_{i=1}^{N} y_i = \sum_{i=1}^{N} K_i \, x_i = 1$$

  (4) If the sum is larger than 1, lower/higher T is needed, and vice versa.

  (5) For dew point, repeat 1-4 with the equation in below for the step 3:

  $$\sum_{i=1}^{N} x_i = \sum_{i=1}^{N} y_i / K_i = 1$$

22.2 Flash distillation

- **Mass balance dictates the following relationship:**

$$x_{F,i} = f\, y_{D,i} + (1 - f)x_{B,i}$$

✓ Assuming that the two phases are in equilibrium,

$$\frac{y_{D,i}}{x_{B,i}} = K_i = \frac{1}{f}\left(\frac{x_{F,i}}{x_{B,i}} + f - 1\right)$$

✓ Just like for the bp/dp estimation, we can solve the eqn iteratively to get final values of T and K_is:

$$\sum_{i=1}^{N} x_{B,i} = 1 = \sum_{i=1}^{N} \frac{x_{F,i}}{f(K_i - 1) + 1}$$

22.3 Fractionating column

- **Unlike in the binary case, we assume # of plates to calculate compositions.**

  ✓ Because of the difficulties and non-idealness, it is almost impossible to specify compositions of all chemicals.

  ✓ Instead, we identify two key components—**light key** (LK), and **heavy key** (HK) compound.

  ✓ One usually chooses the two adjacent (ranked in terms of volatility) chemicals as LK and HK; this practice is called *sharp separation*.

  ✓ One usually specifies $x_{D,H}$ and $x_{B,L}$ for design. The two are usually small/high in value.

22.3 Minimum *N*

- **Minimum number of plates is calculated when R_{Dm} is ?**

$$N_{min} = \frac{\ln\left[\frac{(\frac{x_{D,i}}{x_{B,i}})}{(\frac{x_{D,j}}{x_{B,j}})}\right]}{\ln \alpha_{ij}} - 1$$

What is the eqn.'s name and are the underlying assumptions?

✓ If the α_{ij} changes significantly (> 10%) throughout the column, use

$$\bar{\alpha}_{ij} = \sqrt[3]{\alpha_{D,ij}\alpha_{F,ij}\alpha_{B,ij}}$$

22.3 Minimum R_{Dm}

- **Minimum R_{Dm} is calculated when infinite number of theoretical plates are needed.**

  ✓ We can calculate the value using the equilibrium curve, and operating line between the key components:

$$R_{Dm} = \frac{x_D - y'}{y' - x'}$$

where *x'* and *y'* are the values at the intersection of feed line and eq curve, respectively.

  ✓ If key components make up more than 90% of the feed (saturate liquid), the following eqn can be used:

$$\frac{L_{min}}{F} = \frac{(Dx_{D,i}/Fx_{B,i}) - \alpha_{ij}(Dx_{D,j}/Fx_{F,j})}{\alpha_{ij} - 1}$$

what are physical meaning of the fractions?

22.3 Material balance

- ***N* needed for a specified separation at a selected R can be determined by Lewis-Matheson method.**

  ✓ The amount of all components in the products must be specified.

1. For the top plate, determine T and $x_{i,1}$'s using dp estimation eqn.
2. Use material balance eqn to calculate y_i's for plate 2:

$$y_{i,2}\, V_2 = L_1 x_{i,1} + D\, x_{i,D}$$

3. Can assume equimolar flow or use the enthalpy balance.
4. Repeat the steps 2-3 until the feed plate is reached.
5. Check the feed composition. If different, adjust parameters such as R_{Dm} and/or compositions of the products.
6. Repeat the steps 1-6 starting from the bottom plate to the feed.