#### **Distillation**

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- Distillation is a cascade of flash units.
- The art of distillation dates back to atleast the first century A.D.
- Currently, multistage distillation is by far the most widely used method for separating liquid mixtures of chemical components.
- Distillation is a highly energy intensive technique.

## **Distillation Modeling**



Feed flowrate, *F* Vapor flowrate, *V* Distillate flowrate, *D* Bottoms flowrate, *B* Reflux ratio,  $R = \frac{L}{D}$ 



## **Distillation Modeling**



Consider a distillation unit with N trays and a multicomponent feed  $F_j$  with  $N_c$ components that comes to the *jth* tray and liquid products  $PL_j$  and vapor  $PV_j$ . There could be multiple feed trays and multiple product trays.

- Each tray has a liquid holdup  $M_j$  and a much smaller vapor holdup with liquid and vapor mole fractions  $x_{ij}$  and  $y_{ij}$  respectively.
- Tray j has liquid  $L_j$  and vapor  $V_j$  flowing out of the tray and is connected to streams above and below.
- A mass and energy balance could be written for each component on each tray.



$$- F_j z_{ij} + L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1} - (PL_j + L_j) x_{ij} - (V_j + PV_j) y_{ij} = 0 \qquad i = 1, 2, ..., N_c; \quad j = 1, 2, ..., N$$

Equilibrium Expressions:

$$y_{ij} = K_{ij} x_{ij}$$
$$K_{ij} = K(T_j, P_j, x_{ij})$$

Summation Equations:

$$\sum_{i} x_{ij} = 1, \qquad \sum_{i} y_{ij} = 1, \qquad j = 1, 2, ..., N$$

Heat Balance:

$$F_{j}HF_{j} + L_{j-1}H_{l,j-1} + V_{j+1}H_{v,j+1} - (PL_{j} + L_{j})H_{lj} - (V_{j} + PV_{j})H_{vj} + Q_{j} = 0 \qquad j = 1, 2, ..., N$$

## **MESH Equations**

- The Mass, Equilibrium, Summation, and Heat (MESH) equations form the standard model for tray-by-tray distillation model.
- Note that the thermodynamic properties (K values and specific enthalpies) are expressed as implicit functions that require physical property models.
- These are a large number of equations that are not trivial to solve.
- For this reason, short-cut methods are typically used for designing columns.
- Once a column is designed, its performance is analyzed using a detailed model.

## **Short-cut Distillation Model**

- Light Key: The component that is present in significant quantity in the bottoms stream is called the light key component.
  - Components lighter than the light key can be assumed to come out completely in the distillate steam.
  - Heavy Key: The component that is present in significant quantity in the distillate stream is called the heavy key component.
  - Components heavier than the heavy key can be assumed to come out completely in the bottoms stream.
  - Degrees of Freedom: A column has three degrees of freedom and is fully specified if the following are known:
    - 1. Overhead split fraction of light key ,  $\xi_{lk}$
    - 2. Overhead split fraction of heavy key,  $\xi_{hk}$
    - 3. Column pressure or temperature

#### **Short-cut Distillation Model**

Assumptions:

- Vapor is an ideal gas and the liquid is an ideal solution.
- Each stage is at equilibrium and is modeled as a flash unit.
- $\alpha_{k/n}$  is independent of temperature and pressure.
- The split fractions of the light and heavy keys are known  $(\xi_{lk} \text{ and } \xi_{hk} \text{ are known}).$
- The column is under total reflux.

## **Fenske Equation**

Under the above assumptions, the minimum number of stages is given by the Fenske equation:

$$N = \frac{ln \left[ \frac{(\xi_{lk}(1 - \xi_{hk}))}{(\xi_{hk}(1 - \xi_{lk}))} \right]}{ln(\alpha_{lk/hk})}$$

Once N is known, all other component split fractions can be obtained by substituting k for lk in the Fenske equation. With minor rearrangement:

$$\xi_k = \frac{\alpha_k^N \xi_{hk}}{1 + (\alpha_k^N - 1)\xi_{hk}}$$

### **Selection of column** P or T



Column pressure is lower at the top than at the bottom
More volatile components are higher in concentration at the top

 $T_{cw} \leq T_{bub,C} \leq T_{dew,C} \leq T_{bub,R} \leq T_{dew,C} \leq T_{st}$ 

#### **Selection of column** P or T

Column pressure is selected so that the following constraints hold.

- Select the condenser pressure so that  $T_{bub,C} \ge 310 K$ . This ensures that  $T_{cw} \sim 303 K$ .
- Select condenser pressure so that all bubble point temperatures are below the critical temperature of the mixture.  $T_{bub} \leq T_{cm}$  where  $T_{cm} = \sum x_k T_c^k$ .
- From the bubble point equation we note that  $T_{bub}$ increases with P and we prefer to choose P above 1 atm. Thus  $P = \bar{\alpha}_n P_n^0(T_{bub}) \ge 1 atm$

#### **Partial Condenser and Reboiler**

- The conditions given in the previous slide can be difficult to satisfy when we have non-condensible or non-volatile comonents.
- If there are non-condensibles in the distillate, a partial condenser should be used.
- If there are non-volatiles in the bottoms, a partial reboiler should be used.
- Mass and energy balance calculations for partial condensers and reboilers are greatly simplified by noting that the product streams are saturated liquid and vapor as shown in the next slide.

#### **Partial Condenser Calculations**



Figure 1 is equivalent to Figure 2.

The calculation of flowrates in Figure 2 is a straightforward flash calculation.

 $T_{cond}$  can be easily calculated as *P* is specified and  $\frac{D_v}{D}$  is specified.  $D_v$  is the mole rate of non-condensibles and *D* is the total distillate flowrate.

#### **Total vs. Partial Reboiler**



- The temperature of the stream exiting the reboiler is the highest temperature in the column.
- To avoid excessively high temperatures, a partial reboiler effectively adds an extra equilibrium stage.

#### **Total Reboiler Calculations**



Consider a mixture with three components, 1, 2 and 3 where 2 is the key component in the bottoms stream and 3 is a very high boiling component.

- In a total reboiler, the  $y_1 = x_1$ ,  $y_2 = x_2$  and  $y_3 = x_3$ .
- The dew point temperature can be computed from  $P_2^0(T_{dew}) = P\left(\frac{y_1}{\alpha_{1/2}} + \frac{y_2}{\alpha_{2/2}} + \frac{y_3}{\alpha_{3/2}}\right).$
- Since component 3 has a high boiling point,  $\alpha_{3/2}$  is a very small number and so the dew temperature  $T_{dew}$  will be very high.

### **Partial Reboiler Calculations**



Consider the same mixture as in |the previous slide. In a partial reboiler,  $y_i$  and  $x_i$ are in equilibrium since the reboiler is effectively a flash unit.

- Since component 3 has a very high boiling point, its mole fraction in the vapor stage is expected to be almost zero at reasonable temperatures.
- The dew point temperature can be computed from

$$P_2^0(T_{dew}) = P\left(\frac{y_1}{\alpha_{1/2}} + \frac{y_2}{\alpha_{2/2}}\right).$$

Since the term  $\frac{y_3}{\alpha_{3/2}}$  is negligible, the dew temperature  $T_{dew}$  will not be as high as in a total reboiler.

## **Reflux Ratio and Theoretical Stages**

Calculate the actual theoretical stages and reflux ratio from the following equations (Westerberg correlations)

• 
$$N_i = \frac{12.3}{(\alpha_{lk/hk} - 1)^{2/3}(1 - \beta_i)^{1/6}}$$
  $i = lk, hk$ 

where  $\beta_{lk}$  is the split fraction of the light key at the top  $(\beta_{lk} = \xi_{lk})$  and  $\beta_{hk}$  is the split fraction of the heavy key at the bottom  $(\beta_{hk} = 1 - \xi_{hk})$ .

• 
$$R_i = \frac{1.38}{(\alpha_{lk/hk} - 1)^{0.9}(1 - \beta_i)^{0.1}}$$
  $i = lk, hk$ 

- From  $N_{lk}$  and  $N_{hk}$  calculate the actual theoretical stages as:  $N_T = 0.8max(N_i) + 0.2min(N_i)$
- From  $R_{lk}$  and  $R_{hk}$  calculate the reflux ratio as:  $R = 0.8max(R_i) + 0.2min(R_i)$

# **Design Procedure for Distillation**

