CE407 SEPARATIONS

Lecture 12

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Distillation Column Specifications

- Specify the Feed – composition and quality
  - Binary $\mathbf{x_F}$ and **q** $\mathbf{x_F}$ refers to the light component
    - Mole fraction of heavy component = 1 – $\mathbf{x_F}$
  - Ternary $\mathbf{x_{1F}}$, $\mathbf{x_{2F}}$, and **q**
    - $\mathbf{x_{3F}} = 1 - \mathbf{x_{1F}} - \mathbf{x_{2F}}$
  - Generic **N** components $\mathbf{x_{1F}}$, $\mathbf{x_{2F}}$, $\mathbf{x_{3F}}$, … $\mathbf{x_{N\text{-}1F}}$, and **q**
    - $\boldsymbol{x_{N,F} = 1 - \sum_1^{N-1} x_{i,F}}$
- After specifying the feed you have 4 Degrees of Freedom (things you get to pick…)

Common Examples

(each case could be specified with different variables than these)

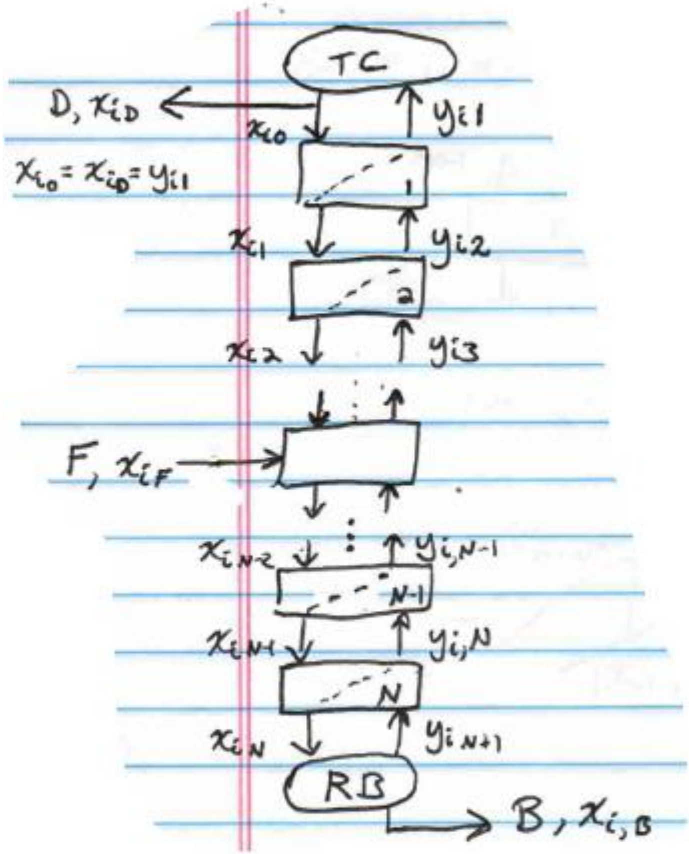
- Binary: $\mathbf{x_D}$, $\mathbf{x_B}$, **R**, Feed Location
- Ternary: $\mathbf{x_{1D}}$, $\mathbf{x_{1B}}$, $\mathbf{x_{3D}}$, **R**
- Once you specified four variables the entire process is determined

Degrees of Freedom

- Look at the Ternary Case
- If we specified $\mathbf{x_{1D}}$, $\mathbf{x_{1B}}$ and $\mathbf{x_{3D}}$
- Then $\mathbf{x_{2D}} = 1 - \mathbf{x_{1D}} - \mathbf{x_{3D}}$
- Now mass balances dictate that
  - **F = D + B**
  - $\mathbf{Fx_{1F} = Dx_{1D} + Bx_{1B}}$
- That is 2 equations and 2 unknowns, therefore D and B are determined and we cannot choose them.
- Mass balance also dictates that
  - $\mathbf{Fx_{3F} = Dx_{3D} + Bx_{3B}}$
  - $\mathbf{x_{3B}}$ is the only unknown, so it is now determined
- We now have flow rates and composition of Feed, Distillate, and Bottoms
- **We must not over-specify the system or it may not be solvable!**

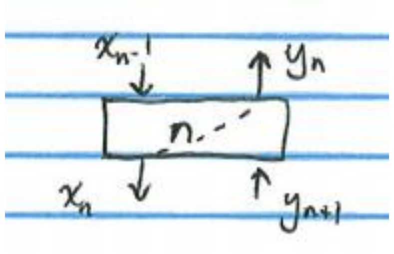
Multi-component Distillation

- Notice that now all of the mole fractions carry a subscript designating which component as well as what stage that flow is leaving
- A mass balance can be done for each component leading to a collection of Operating Lines
- $y_{i,n+1} = \frac{R}{R+1} x_{i,n} + \frac{x_{i,D}}{R+1}$ Rectifying Line for Component i
  - $R = {}^{L}/_{D}$
- $y_{i,n+1} = \frac{S+1}{S} x_{i,n} - \frac{x_{i,B}}{S}$ Stripping Line for Component i
  - $S = {}^{\overline{V}}/_{B} = \frac{D}{B}(R+q) + q - 1$
- We will limit our discussion to constant molar flows

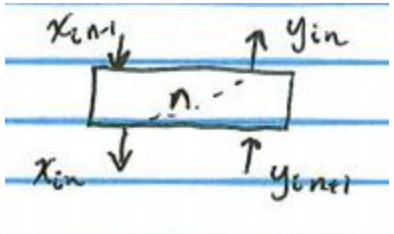


Detailed Multi-component Distillation Calculations

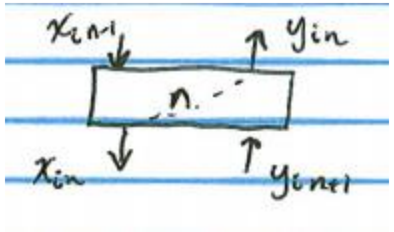
- We will start by comparing Binary calculations to Multi-component
- Binary
  - Calculate one set of Operating Lines
  - $\mathbf{x_n}$ is related to $\mathbf{y_{n+1}}$ via OP Line
  - $\mathbf{x_n}$ is related to $\mathbf{y_n}$ via Equilibrium Curve



- Multi-component
  - We need to include subscripts for the component
  - Calculate a set of Operating Lines for each component
  - $\mathbf{x_{i,n}}$ is related to $\mathbf{y_{i,n+1}}$ via OP Line for specific component
  - Equilibria Calculations – must include all components in calculation
    - When working downward in column use DEW POINT calculation to determine $\mathbf{x_{i,n}}$ from $\mathbf{y_{i,n}}$
    - When working upward in column use BUBBLE POINT calculation to determine $\mathbf{y_{i,n}}$ from $\mathbf{x_{i,n}}$



Bubble and Dew Point Calculations



- Working Down the Column
- We know $\mathbf{x_{i,o}}$ and $\mathbf{y_{i,1}}$ from $\mathbf{x_{i,D}}$
- We use Dew Point calculation to get $\mathbf{x_{i,1}}$ from $\mathbf{y_{i,1}}$
- $\sum_{i=1}^{N} x_{i,n} = \sum_{i=1}^{N} \frac{y_{i,n}}{k_{i,n}} = 1.0$
- $k_{i,n}$ is $\frac{P_i^{sat}}{P}$ for ideal case
- Then the rectifying OP Lines are used to relate $\mathbf{y_{i,n+1}}$ to $\mathbf{x_{i,n}}$
- Continue Down step by step
- Working Up the Column
- We use Bubble Point calculation to get $\mathbf{y_{i,n}}$ from $\mathbf{x_{i,n}}$
- $\sum_{i=1}^{N} y_{i,n} = \sum_{i=1}^{N} k_{i,n}\, x_{i,n} = 1.0$
- Then the stripping OP Lines are used to relate $\mathbf{x_{i,n-1}}$ to $\mathbf{y_{i,n}}$
- Continue Upward step by step

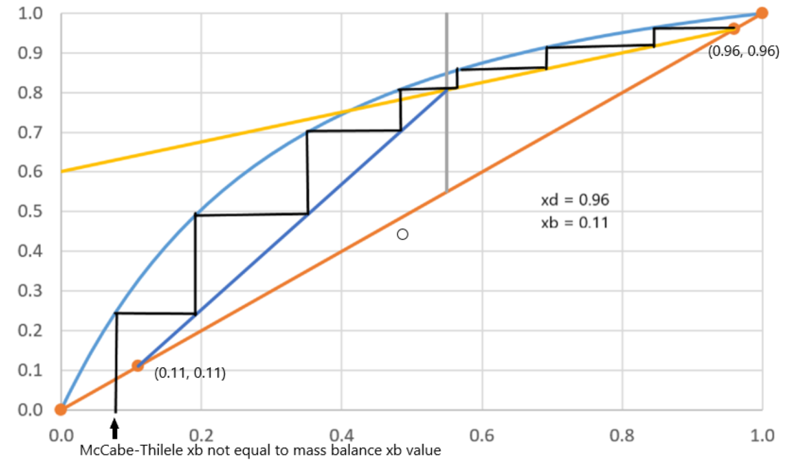
Detailed Multi-Component Distillation Calculations

- The reason we work from both ends is that we do not where the feed is going to enter (we don't know how many stages we have) and therefore we do not know when to switch from R OP Line to S OP Line
- The two series of calculations will eventually cross one another. That is the feed stage
- We can add the number of R stages and S stages at the crossing point to get the total number of stages
- Practically we use commercial Process Simulation Software
- Unisim is really amazing and you will learn to use it in CE 408!

Performance Calculations

- We have been doing design models so far
  - We have a desired separation and are determining what number of stages, reflux ratio, and feed location are required to achieve it
- What if we have a column and want to know what it will do?
  - Given a certain feed, # of stages, reflux ratio, feed location plus one more (S or D, perhaps) what will the compositions of D and B actually be?
- Unisim will calculate flows, compositions, temperatures
  - It won’t work if you over-specify the system

Performance Calculations

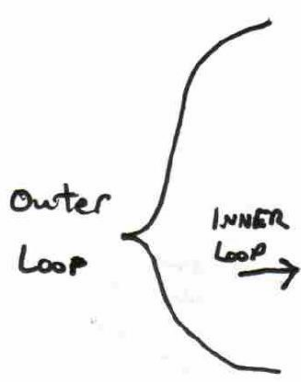


Binary Example

- Guess a value for $\mathbf{x_D}$
- Use mass balance based on the feed and this $\mathbf{x_D}$ to determine what $\mathbf{x_B}$ would be
- Calculate operating lines from R, $\mathbf{x_D}$, and feed information
- Draw in the number of stages that the column actually has
- Determine $\mathbf{x_{B\ obtained}}$ from McCabe-Thiele
- If $\mathbf{x_{B\ obtained}}$ does not match $\mathbf{x_B}$ from material balance then the $\mathbf{x_D}$ was incorrect
- Adjust $\mathbf{x_D}$ and iterate until $\mathbf{x_{B\ obtained}}$ matches $\mathbf{x_B}$
- You want them to match quite well because we are trying to determine what the compositions are that we will get
    - Before we were trying to determine how many stages we need to meet or beat a purity specification

Performance Calculations

Multi-Component Example



- Program chooses values for $\mathbf{x_{iD}}$
- Mass balance calculations based on this $\mathbf{x_{iD}}$ to determine what $\mathbf{x_{iB}}$ would be
- Tray to tray calculations determine $\mathbf{x_{iB\ obtained}}$
- If $\mathbf{x_{iB\ obtained}}$ does not match $\mathbf{x_{iB}}$ from material balance then adjust $\mathbf{x_{iD}}$ and iterate until $\mathbf{x_{iB\ obtained}}$ matches $\mathbf{x_{iB}}$

- One can use a simulator to get a design by specifying column and then use inner and outer loop to determine outputs. Then one can make adjustments to the specifications until they are satisfied with the result

Extremely (Embarrassingly) Rough Multi-Component Short Cut

- If LK and HK represent a substantial portion of the feed…
- Perform a McCabe-Thiele analysis treating the case as a binary mixture of the LK and HK
- This gives an estimate of the number of stages and the feed location
- This estimate **MUST** be presented as a very low confidence starting point for the design