CE407
SEPARATIONS

Lecture 09

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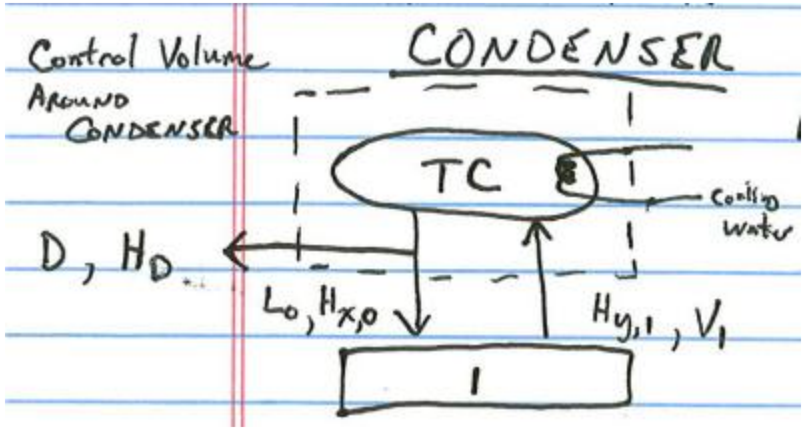
Continuous Distillation – Enthalpy Balances

McSH pp 694-701, pp 679, 682 eq 21.1 and 21.2

- How much energy does one need to remove via condenser and add via reboiler?
- Condenser
- Control Volume

  around condenser

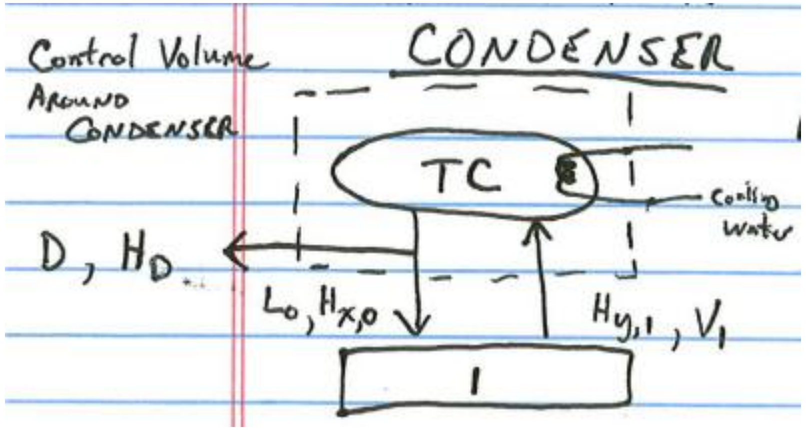


- Heat added = Enthalpy out – enthalpy in

$$-q_c = DH_D + L_0H_{x,0} - V_1H_{y,1}$$
$$= (D + L_0)H_{x,0} - V_1H_{y,1}$$

- Note: $\mathbf{q_c}$ is defined as the amount of heat **REMOVED** via the condenser and is a positive number. The enthalpy balance is the amount of heat added, therefore the term appears as $\mathbf{-q_c}$ in the equation. The fact that $\mathbf{-q_c}$ is therefore a negative term is consistent with the fact that we are removing heat to affect a phase change from vapor to liquid

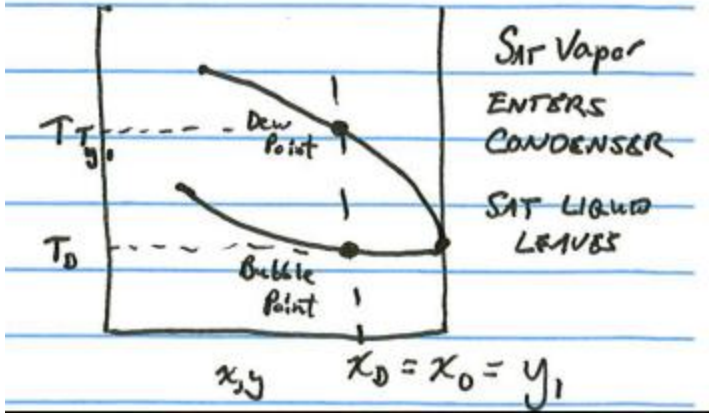
Enthalpy Balances: Condenser, continued



- $-q_c = (D + L_0)H_{x,0} - V_1 H_{y,1}$
- But from mass balance we know that $V_1 = D + L_0$
- $-q_c = (D + L_0)H_{x,0} - (D + L_0)H_{y,1}$
- And from definition of reflux ratio **$L_0 = D R$**

$$\boxed{-q_c = D(1 + R)\left(H_{x,0} - H_{y,1}\right)}$$

- It's not as simple as just looking at Heats of Vaporization
- You have the temperature changing from Dew Point to Bubble Point
- Heats of Vaporization are defined for a pure material at a given temperature (usually the normal boiling temperature for pure material) and we are condensing over a range of temperatures



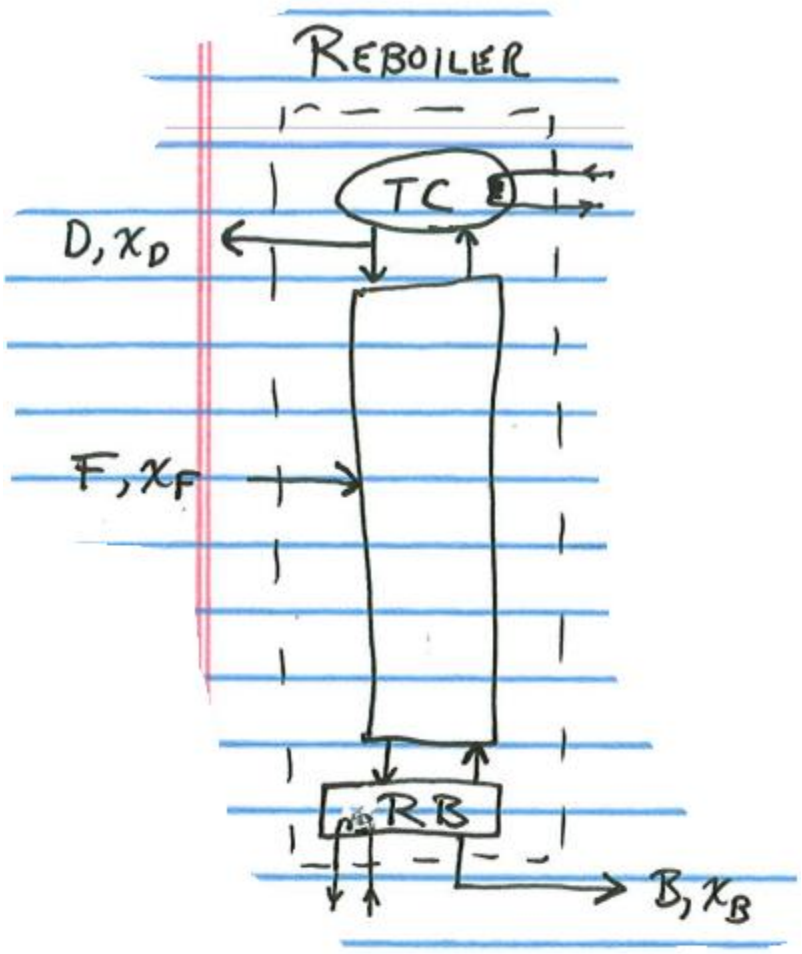
Enthalpy Balances: Reboiler

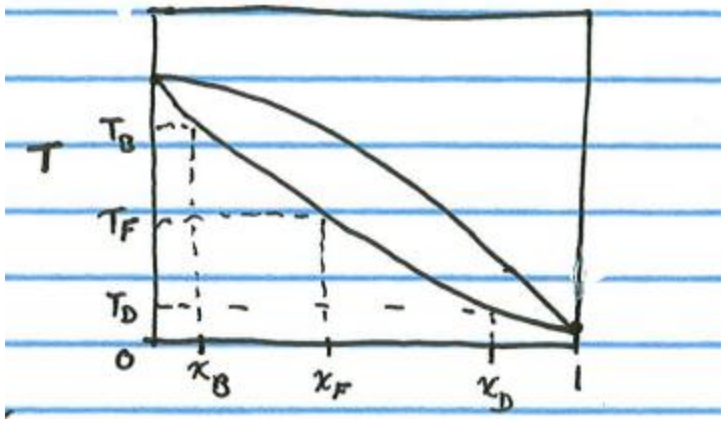
- Set up Control Volume around entire column

Heat added = Enthalpy out – enthalpy in

$$\boxed{q_r - q_c = DH_D + BH_B - FH_F}$$

- q_r is defined as heat ADDED via the Reboiler and is a positive number
- We will need to determine the temperature of each stream in order to calculate enthalpies





Txy diagram for saturated liquid feed case

Enthalpy Balances

- We have the temperature and composition of all streams
  - Calculate enthalpy of each stream
  - Start with enthalpy balance around condenser
    - Solve for $\boldsymbol{q_c}$
  - Next evaluate enthalpy balance around entire column
    - Solve for $\boldsymbol{q_r}$

Enthalpy Balances – Heat Loads

Condenser

- Use q_c to determine rate of cooling water required for condenser

$$\boxed{q_c = \dot{m}_{cw} C^L_{p\,H_2O}(T_{out} - T_{in})}$$

  - Where $\dot{m}_{cw}$ is mass flow rate of cooling water
  - $C^L_{p\,H_2O}$ is the heat capacity of liquid water
    - Typically $C^L_{p\,H_2O} \approx 1\ \frac{cal}{g\,°\mathrm{C}}$
  - T_{in} is the incoming temperature of the cooling water
  - T_{out} is the outgoing temperature of the cooling water
    - this may be limited by thermal pollution concerns
    - of course, you don’t want this stream to reach a boiling temperature

Enthalpy Balances – Heat Loads

Reboiler

- Use q_r to determine rate of steam consumption required for reboiler

$$\boxed{q_r = \dot{m}_{steam}\,\Delta H^{vap}_{H_2O}}$$

  - Where $\dot{m}_{steam}$ is mass flow rate of steam
  - $\Delta H^{vap}_{H_2O}$ is the heat of the steam phase change
- This equation assumes steam enters as saturated vapor and exits as saturated liquid – consult steam tables for enthalpy change of steam that has varying quality values

	T (°C)	$P^{sat}_{H_2O}(kPa)$	$\Delta H^{vap}_{H_2O}\left(\frac{kJ}{kg}\right)$
	100	101.3	2257
~150 # steam	188	1200	1986

Enthalpy Balance Example

- A 100 mole/hr feed of 40 mole percent n-pentane and 60 mole percent n-heptane enters a continuous distillation tower operating at a reflux ratio $R_D = 0.4$
- The column is fitted with a total condenser. The mole fraction, x_D, of n-pentane in the distillate is 0.95 and in the bottom product the mole fraction of n-pentane, x_B, is 0.05. Feed enters as a saturated liquid.
  a. Generate expressions for the enthalpies of Liquid mixtures, $H_x(T, x)$, and Vapor mixtures, $H_y(T,y)$ of n-pentane and n-heptane.
  b. Calculate the required rate of heat removal from the condenser, q_c, and required rate of heating at the reboiler, q_r.
  c. Calculate the required flow rates of cooling water to the condenser and steam to the reboiler.

Property	Value for n-pentane	Value for n-heptane
Normal boiling point in K	309.20	371.57
Cp of liquid in J/(mol K)	168	226
Cp of vapor in J/(mol K)	120	188
DH^{vap} at normal boiling point in kJ/mol	26.40	31.77

Enthalpy Balance Example

- Define reference states such that the liquid enthalpy is zero for each pure component at 309.2 K.

Liquid Phase Enthalpy

- $H_{xi}(T) = C_{pi}^{L} * (T - T_{nb1})$
- $H_{x\,pentane}(T) = 168 * (T - 309.2)$
- $H_{x\,heptane}(T) = 226 * (T - 309.2)$
- $H_x(T, x) = x * H_{x1}(T) + (1 - x) * H_{x2}(T)$
- $H_x(T, x) = x * \left(168 * (T - 309.2)\right) + (1 - x) * \left(226 * (T - 309.2)\right)$
- $H_x(T, x) = (226 - 58x) * (T - 309.2)$ H_x in $\frac{J}{mol}$ T in **K**

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Enthalpy Balance Example

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Vapor Phase Enthalpy

- $H_{y1}(T) = \Delta H_1^{vap}(T_{nb1}) + C_{p1}^V * (T - T_{nb1})$
- $H_{y2}(T) = C_{p2}^L * (T_{nb2} - T_{nb1}) + \Delta H_2^{vap}(T_{nb2}) + C_{p2}^V * (T_{nb1} - T_{nb2}) + C_{p2}^V * (T - T_{nb1})$
- $H_{y\,pentane}(T) = 26,400 + 120 * (T - 309.2)$
- $H_{y\,heptane}(T) = 226 * (371.57 - 309.2) + 31,770 + 188 * (309.2 - 371.57) + 188 * (T - 309.2) = 34140.1 + 188 * (T - 309.2)$
- $H_y(T, y) = y * H_{y1}(T) + (1 - y) * H_{y2}(T)$
- $H_y(T, y) = y * [26,400 + 120 * (T - 309.2)] + (1 - y) * [34140.1 + 188 * (T - 309.2)]$
- $H_y(T, y) = 34140.1 - 7740.1\,y + (188 - 68.0\,y) * (T - 309.2)$ H_y in $\frac{J}{mol}$ T in **K**

Enthalpy Balance Example

Required Heating and Cooling Loads

- Temperatures can also be read off of T_{xy} diagram
    - More accurate temperatures can be obtained by using GoalSeek to get exact mole fractions of feed, distillate, and bottoms
- Temperature of Distillate/x_0 is that of saturated liquid at x = 0.95 and is 311 K
- Temperature of Vapor entering condenser is that of saturated vapor at y = 0.95 and is 318 K
- Temperature of Feed is that of saturated liquid at x = 0.40 and is 332 K
- Temperature of Bottoms is that of saturated liquid at x = 0.05 and is 364 K

Note that our Antoine equations did not give us the exact same normal boiling points as quoted in the problem statement. You will find that different sources do not always agree exactly. The values are within 0.01 °C, so let's agree to not worry about the discrepancy.

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Normal boiling point in K	309.20	371.57
Cp of liquid in J/(mol K)	168	226
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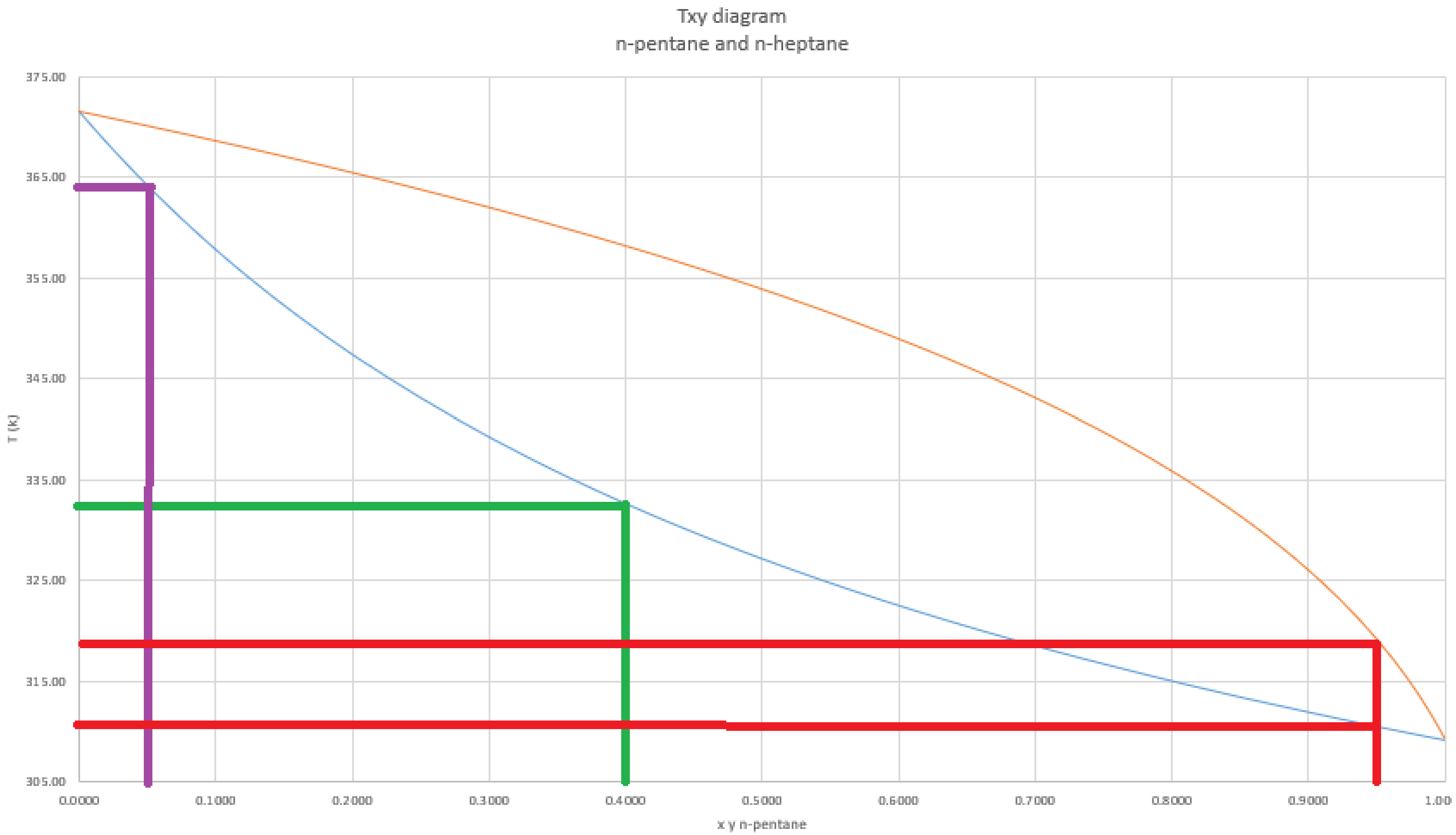
Enthalpy Balance Example



Enthalpy Balance Example

- $H_{x\,0} = H_D = H_x(311, 0.95) = (226 - 58 * 0.95) * (311 - 309.2) = 307.6$ H_x in $\frac{J}{mol}$ T in **K**
- $H_{y\,1} = H_y(318, 0.95) = 34140.1 - 7740.1 * 0.95 + (188 - 68.0 * 0.95) * (318 - 309.2) = 27{,}872.9$ H_y in $\frac{J}{mol}$ T in **K**
- $H_F = H_x(332, 0.40) = (226 - 58 * 0.40) * (332 - 309.2) = 4623.8$ H_x in $\frac{J}{mol}$ T in **K**
- $H_B = H_x(364, 0.05) = (226 - 58 * 0.05) * (364 - 309.2) = 12{,}225.9$ H_x in $\frac{J}{mol}$ T in **K**

Enthalpy Balance Example

- Total Mole Balance: $F = D + B$
- Pentane Mole Balance: $x_F F = x_D D + x_B B$
- $x_F = 0.40$, $F = 100$ mol/hr, $x_D = 0.95$, $x_B = 0.05$
- Solves for: **D = 38.89 and B = 61.11 mol/hr**

Enthalpy Balance Example

- $-q_c = D(1+R)\left(H_{x,0} - H_{y,1}\right)$
- $-q_c = 38.89 * (1+0.4) * (307.6 - 27{,}872.9)$
- $q_c = 1.501 * \ 10^6 \ \frac{J}{hr} = 1.501 * \ 10^3 \ \frac{kJ}{hr}$

- $q_r - q_c = DH_D + BH_B \ - FH_F$
- $q_r - 1.501 * \ 10^6 = 38.89 * 307.6 + 61.11 * 12{,}225.9 \ - 100 * \ 4623.8$
- $q_r = 1.798 * \ 10^6 \ \frac{J}{hr} = 1.798 * \ 10^3 \ \frac{kJ}{hr}$

Enthalpy Balance Example

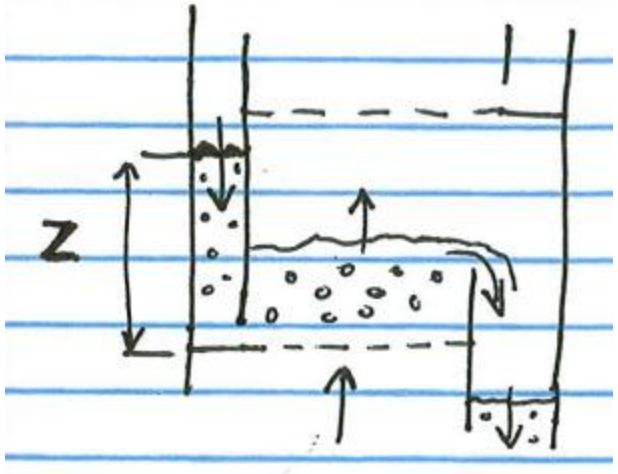
- Cooling water requirement
- 1 BTU/(lb F) = 4186.8 J/(kg C)
- q_c = (mass flow cooling water) * $C_{p,\ water}$ * $(T_{out} – T_{in})$
- $1.501 * 10^6$ J/hr = **m** * 4186.8 J/(kg C) * 10 C
- **$m_{cooling\ water}$ = 35.9 kg/hr**

- Steam Requirement
- q_r = (mass flow steam) * DH^{vap}_{steam}
- $1.798 * 10^3$ kJ/hr = **m** * 1986 kJ/kg
- **m_{steam} = 0.9 kg/hr**

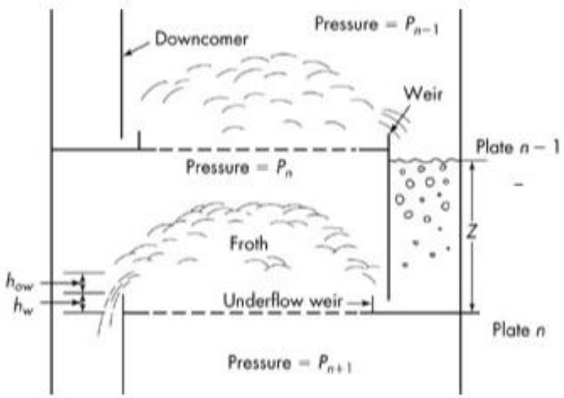
Continuous Distillation – Tower Design

McSH pp 701-712

Design of Sieve Plate Trays

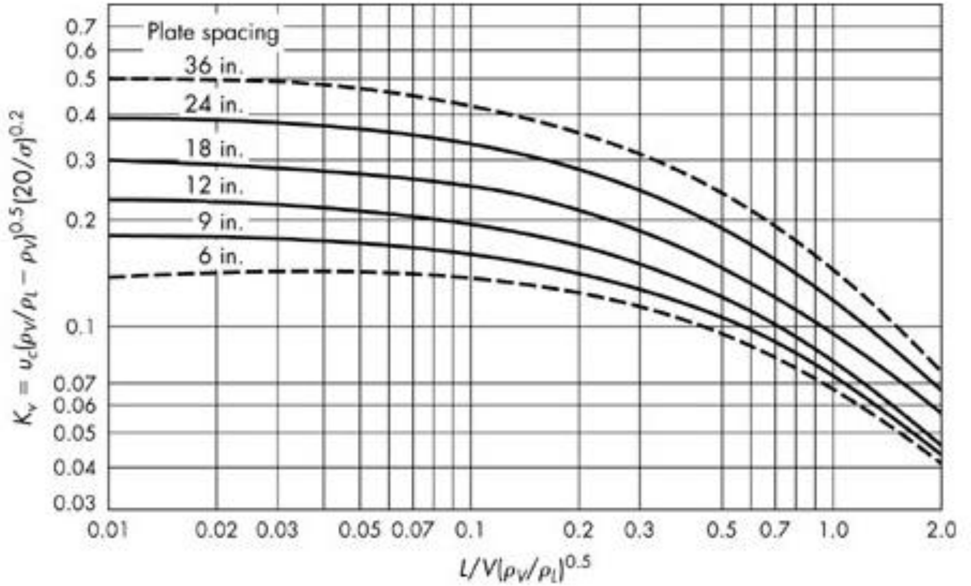


- Pressure increases as you progress down the tower
- The pressure is needed to motivate the vapor through the holes in the tray and through the liquid held up on the tray
- Due to the ΔP, a column of liquid is held up in the downcomer (similar to a monometer) of height **Z**
- The text discusses methods for calculating **Z**, but we won't touch on it at this point
- The important point is that if **Z** exceeds the distance to the weir on the plate immediately above then the column experiences **FLOODING** and the plates won't function properly
- The diameter of the column must be specified such that the vapor velocity does not exceed the **"Flooding Velocity"**



Flooding

- Figure 21.26 in McSH: Note that this is a log-log graph!
- Choose curve corresponding to your tray spacing
- Calculate $\frac{L_{mass}}{V_{mass}}\sqrt{\rho_V/\rho_L}$
  - Note that **L** and **V** are MASS flow rates
  - Note that $\boldsymbol{\rho_V}$ and $\boldsymbol{\rho_L}$ are MASS densities
  - **L/V** we have used in the past were molar flows
- Find $\boldsymbol{K_V}$ from chart
- Use equation 21.68 to calculate flooding velocity



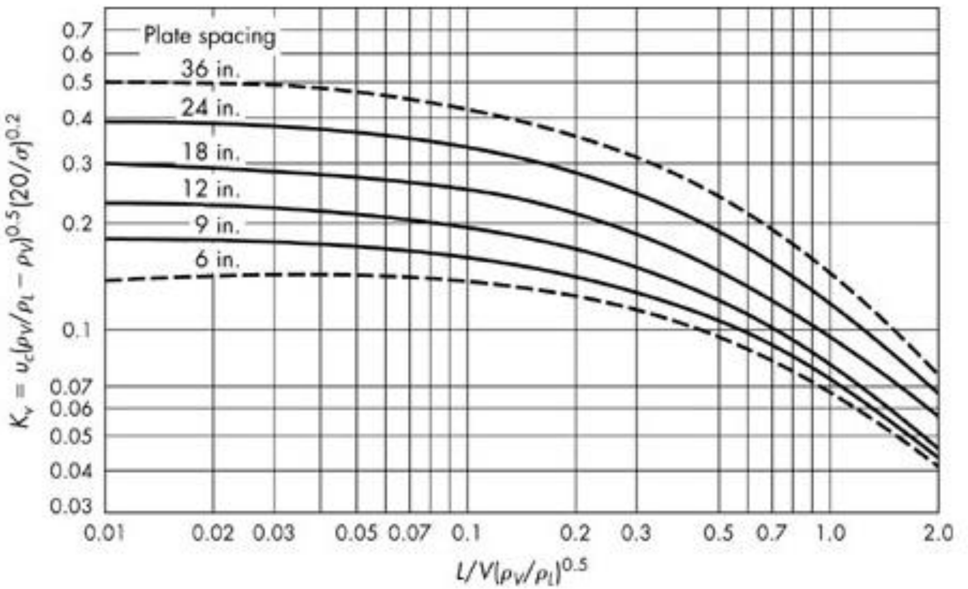
$$u_c = u_{flooding} = K_V\sqrt{\frac{\rho_L - \rho_V}{\rho_V}}\left(\frac{\sigma}{20}\right)^{0.2}$$

- σ is the surface tension in dyn/cm, **u** is in ft/s on this graph
- A given chart will correspond to **u** in ft/s or m/s: *be sure you know which it is!*

Flooding

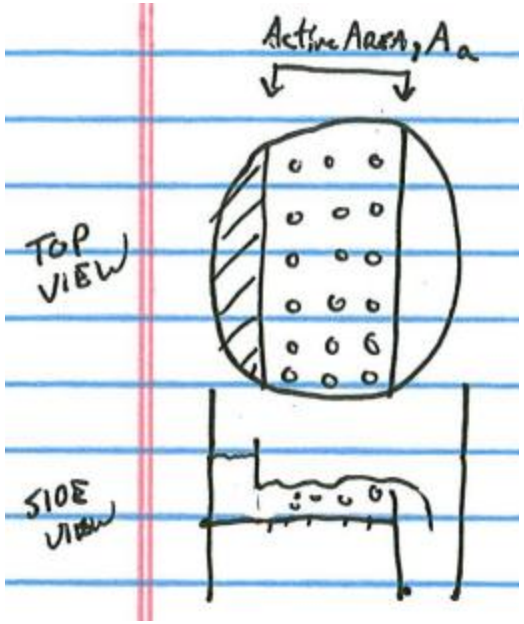
- Calculate $\frac{L_{mass}}{V_{mass}}\sqrt{\rho_V/\rho_L}$
  - Note that **L** and **V** are MASS flow rates
  - Note that $\boldsymbol{\rho_V}$ and $\boldsymbol{\rho_L}$ are MASS flow densities
  - **L/V** we have used in the past were molar flows

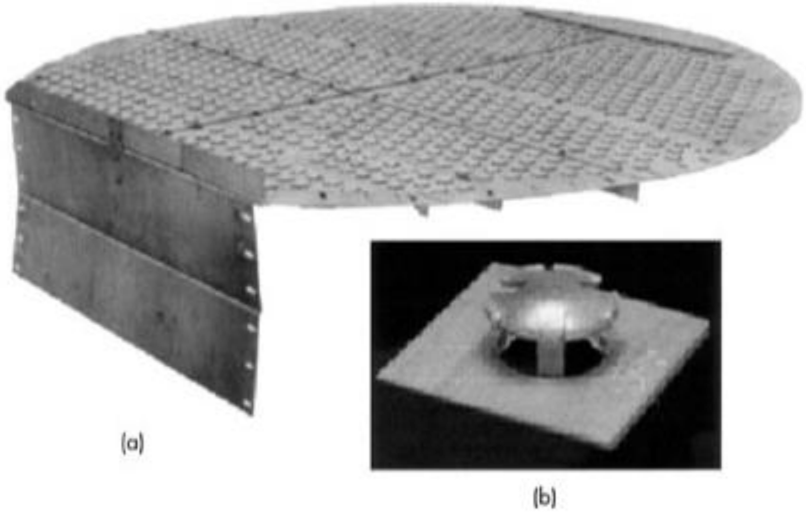
  - $\frac{L_{mass}}{V_{mass}} = \frac{L\,\overline{MW_L}}{V\,\overline{MW_V}}$
  - When we are evaluating at the top of the tower the flows are often close to pure light component and $\overline{MW_L} \approx \overline{MW_V}$
  - Therefore $\frac{L_{mass}}{V_{mass}} \approx \frac{L}{V}$
  - $\frac{L}{V} = \frac{R}{R+1}$ can be used for $\frac{L_{mass}}{V_{mass}}$ as long as we are aware that it only applies when $\overline{MW_L} \approx \overline{MW_V}$



Flooding, Continued

- Now we have a value for the a vapor velocity that will cause flooding.
- We will add a safety factor because we don't want to operate on the edge of flooding conditions
    - Various sources use different factors, let's choose $u \approx 0.7u_{flood}$
- Most of the plate is covered by holes
- $\boldsymbol{A = Total\ Area = \frac{\pi D^2}{4}}$
- Downcomer, etc cover 15% of total area
- Net area for flow = **0.85A**





Flooding, Continued

$$V = u\,A_n \frac{P}{RT}$$

Molar vapor flow = (volumetric flow) * (moles/volume)

- From ideal gas law PV = nRT you get $\frac{P}{RT} = \frac{n}{V} = \frac{moles}{Volume}$
- In this context V is just a volume

- $A_n = 0.85\frac{\pi D^2}{4}$ net area for flow
- Steps
  - Calculate u_{flood} and apply safety factor
  - Use molar flow rate V to calculate A_n
  - Calculate required column diameter

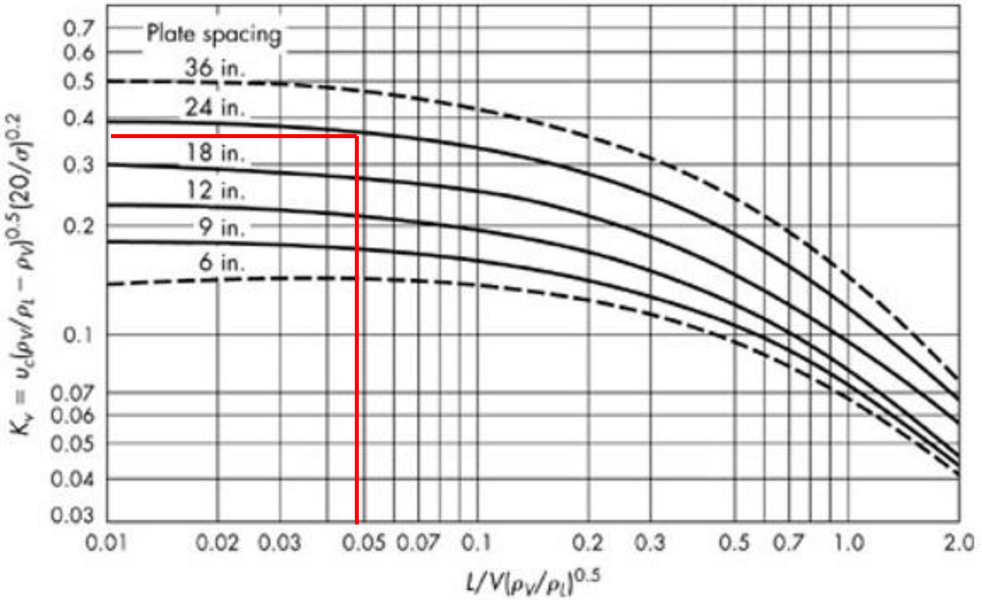
- **Note: Column is most susceptible to flooding at the top of the tower. Use conditions corresponding to the top of the tower in this evaluation!**

Flooding Example

- We have a distillate flow rate of 3259 mol/minute of CCl_4 (light) and C_8H_{18} (heavy)
    - $x_D = 0.859$
- Reflux ratio = 2.55, Tray Spacing = 24”
- Flooding velocity is calculated at TOP of tower
- Problem Statement indicates that we should assume densities of the liquid and vapor to be that of pure CCl_4
    - Liquid density: $\rho_L = 1490\ \frac{kg}{m^3}$
- Vapor density: By the Ideal Gas Law we can calculate molar volume
- $$V = \frac{RT}{P} = \frac{83.14\frac{bar\ cm^3}{mol\ K}(273.15+76.75)\ k}{1.013\ bar} = 2.872 * 10^4\ \frac{cm^3}{mol}$$
    - Then the mass density can be calculated as
    - $$\rho_V = \frac{1\ mol}{2.872 * 10^4\ cm^3} * \frac{153.823\ g}{mol} * \frac{kg}{1000\ g} * \frac{10^6 cm^3}{m^3} = 5.34\ \frac{kg}{m^3}$$
        - MW CCl_4 = 153.823

Flooding Example

- Near the top of the tower (where the mole fractions are near 1.0), the average molecular weight of the liquid and the vapor are approximately equal at any location
  - At the top of the tower $\frac{L_{mass}}{V_{mass}} = \frac{L*MW_L}{V*MW_V} \approx \frac{L}{V} = \frac{R}{R+1} = \frac{2.55}{2.55+1} = \mathbf{0.718}$



- $\frac{L_{mass}}{V_{mass}}\sqrt{\frac{\rho_V}{\rho_L}} = \mathbf{0.718}\sqrt{\frac{5.34\,\frac{kg}{m^3}}{1490\,\frac{kg}{m^3}}} = \mathbf{0.043}$
- $K_V = u_c\sqrt{\frac{\rho_V}{\rho_L-\rho_V}}\left(\frac{20}{\sigma}\right)^{0.2} = 0.37$
- Unless your surface tension is very different from water, the surface tension factor can be ignored
- $u_c = u_{flooding} = K_V\sqrt{\frac{\rho_L-\rho_V}{\rho_V}} = 0.37\sqrt{\frac{1490-5.34}{5.34}} = 6.17\ \frac{ft}{s}$

Flooding Example

- Vapor volumetric flow rate:
- V molar flow rate $V = L + D = (R+1)D = 3.55 * \ 3259 \ \frac{mol}{min} = 11{,}569 \ \frac{mol}{min}$
- Molar density $\rho_V = \frac{P}{RT} = \frac{1.013 \ bar}{83.14 \frac{bar \ cm^3}{mol \ K} (273.15+76.75) \ k} = 3.482 * \ 10^{-5} \frac{mol}{cm^3} * \frac{10^6 \ cm^3}{m^3} = 34.82 \frac{mol}{m^3}$
- $Q = \frac{V}{\rho_V} = \frac{11{,}569 \frac{mol}{min}}{34.82 \frac{mol}{m^3}} = 332.2 \ \frac{m^3}{min} * \frac{min}{60 \ s} = 5.54 \ \frac{m^3}{s} * \left(\frac{ft}{0.305 \ m}\right)^3 = 195.3 \ \frac{ft^3}{s}$

Flooding Example

- **Column diameter:**
- $Q = A_n * u = 0.85\frac{\pi D^2}{4} * u$
  - (Volumetric flow rate = Area * velocity)
- Column is to operate at 50% of flooding velocity:
- $u = 0.5 * u_{flooding} = 0.5 * 6.17\frac{ft}{s} = 3.09\frac{ft}{s}$
- $Q = 195.3\frac{ft^3}{s} = 0.85\frac{\pi D^2}{4} * 3.09\frac{ft}{s} = 2.06\frac{ft}{s} * D^2$
- $D^2 = \frac{195.3\frac{ft^3}{s}}{2.06\frac{ft}{s}} = 94.67\, ft^2$
- $\boldsymbol{D = 9.7\, ft}$