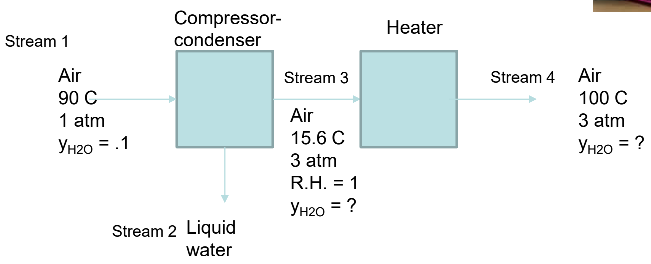
Dean's Lecture

- 11 am tomorrow
- JSB Auditorium
- Counts for one of two lectures required in this class
- Be there early to get a seat!

Professional Program Application

- Required in order to get an add code for ChEn 374 (Fluid Dynamics)
- We will discuss this **after Exam 2**
- You will need to see your faculty advisor
  - – Course planning worksheet completed
  - – Discuss grades in major courses
  - – Ask for advice
- **Due November 18**

HW Review

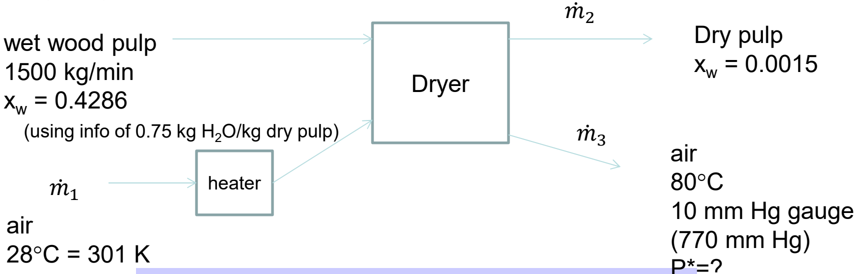


1. Use a basis of 100 moles of moist air entering compressor
2. Find $y_{H2O,3}$ from vapor pressure, RH_3, and definition of partial pressure
3. Note that $y_{H2O,3} = \frac{n_{H2O,3}}{n_{H2O,3}+n_{dry\ air}}$, so if you know $y_{H2O,3}$ and $n_{dry\ air}$, you can get $n_{H2O,3}$
4. Do the balances on moles of water in and out of compressor
5. Use ideal gas law to get ratios of volumetric flow rates

Photo from http://headinthesandblog.org/2016/11/parents-enough-hours-day-much-homework/

17.3. A hot-air dryer is used to reduce the moisture content of 1500 kg/min of wet wood pulp from 0.75 kg H_2O/kg dry pulp to 0.15 wt% H_2O. Air is drawn from the atmosphere at 28°C, 760 mm Hg, and 50% relative humidity, sent through a blower-heater, and then fed to the dryer. The air leaves the dryer at 80°C and 10 mm Hg (gauge). A sample of the exit air is drawn into a chamber containing a mirror and cooled slowly, keeping the gauge pressure at 10 mm Hg. A mist is observed to form on the mirror at a temperature of 40.0°C.

(a) What is the vapor pressure of H_2O at the conditions in the dryer exit?
(b) Calculate the partial pressure and mole fraction of H_2O in the air leaving the dryer.
(c) Calculate the mass of water removed from the pulp (kg/min) and the volumetric flow rate of air entering the system (m^3/min).



Strategy:
1. $P^*_{out,3}$ at 40°C is dew point (from table) = F
2. Get $y_{w,out,3}$ from P_{H2O}/P_{tot} in the 40°C samp
3. Get $y_{H2O,in,1}$ from RH_{in}
4. Balances on
    1. dry pulp mass
    2. moles of water
    3. moles of dry air

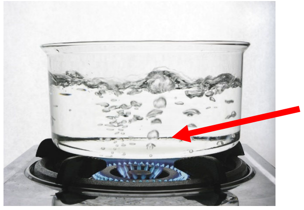
From cooled sample, P*=55.324 mm Hg at 40 C, so $y_{H2O,3}$ = 55.324/770 = .07185, which is the same $y_{H2O,3}$ at 80C!
RH = $y_{H2O}P_{tot}/P^*$(80 C) = .07185*770/355.1 = .156, or 15.6% RH in stream 3

Review

For a vessel with pure H_2O at 10 bar and 100°C

- What is the vapor pressure? $P^*_{H2O} = 1$ atm
- How much vapor is there?

0% vapor since it is pure H_2O and $P_{tot} > P^*_{H2O}$



What is the composition of the gas in the bubbles?

100% water vapor

How could you use Raoult's Law to find the temperature of the bubbles, given a total pressure?

Since $P = P^*_{H2O}$ at this interface (pure H_2O), find T where $P^*_{H2O} = P_{tot}$

Review

One morning the weatherman said that the temperature was 34°F and the dew point was 33°F.

What does this mean? 1°F superheat

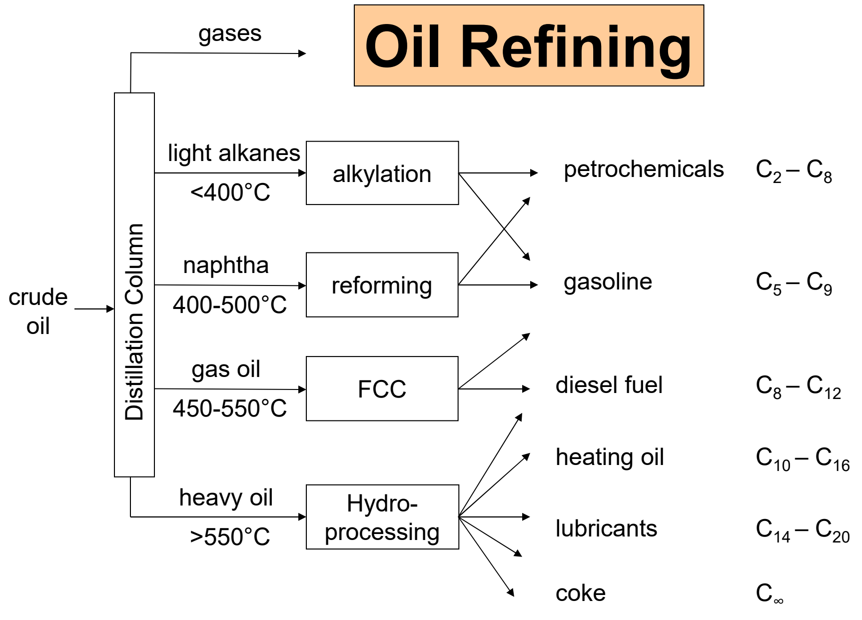
Relative Humidity was reported as 99%.

Class 19

Multicomponent Vapor-Liquid Equilibrium

- Why Multicomponent?
- Review Raoult's Law
- Henry's Law
- Dew Point Calculation
- Bubble Point Calculation
- Flash Calculation

Oil Refining



gases

crude oil

Distillation Column

light alkanes <400°C

naphtha 400-500°C

gas oil 450-550°C

heavy oil >550°C

alkylation

reforming

FCC

Hydro-processing

petrochemicals $C_2 – C_8$

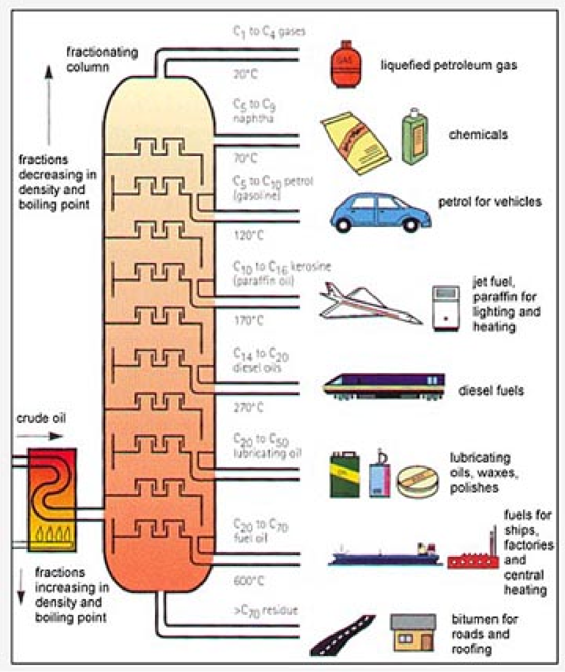
gasoline $C_5 – C_9$

diesel fuel $C_8 – C_{12}$

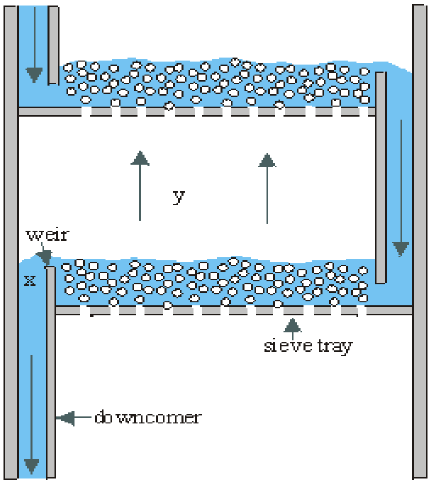
heating oil $C_{10} – C_{16}$

lubricants $C_{14} – C_{20}$

coke C_∞


C_1 to C_4 gases
fractionating column
liquefied petroleum gas
20°C
C_5 to C_9 naphtha
chemicals
fractions decreasing in density and boiling point
70°C
C_5 to C_{10} petrol (gasoline)
petrol for vehicles
120°C
C_{10} to C_{16} kerosine (paraffin oil)
jet fuel, paraffin for lighting and heating
170°C
C_{14} to C_{20} diesel oils
diesel fuels
270°C
crude oil
C_{20} to C_{50} lubricating oil
lubricating oils, waxes, polishes
C_{20} to C_{70} fuel oil
fuels for ships, factories and central heating
600°C
fractions increasing in density and boiling point
$>C_{70}$ residue
bitumen for roads and roofing

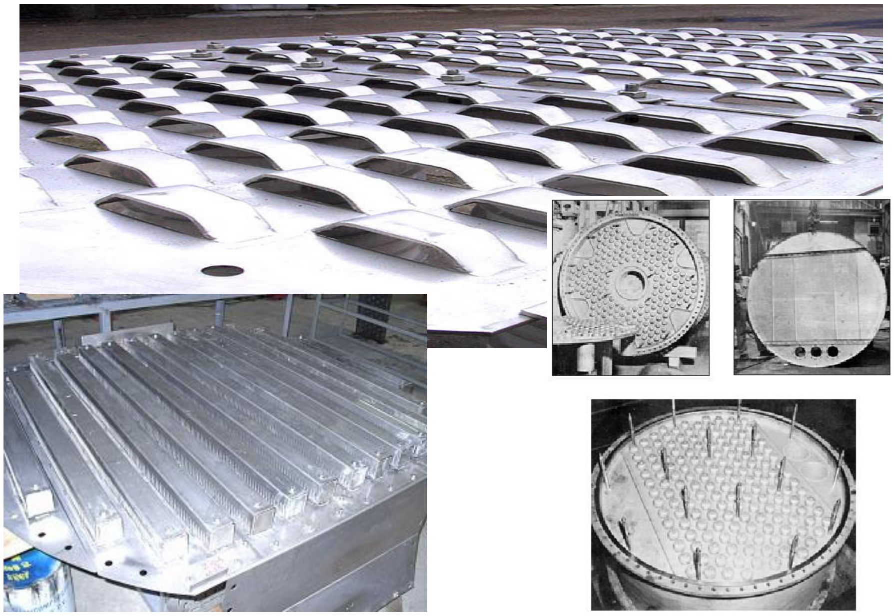
Distillation Column Trays



- On each tray, mixing is high enough to approach vapor-liquid equilibrium
- Vapor is enriched in more volatile component
- Liquid is enriched in less volatile component
- Multiple trays used to achieve greater separation yields

https://www.youtube.com/watch?v=bzAjbwiasfE

Trays in Distillation Column



Henry’s Law

(in place of Raoult’s Law)

- Raoult’s Law when $x_i \rightarrow 1$
  - $P_i = x_i P_i^*$
- Henry’s Law used when $x_i \rightarrow 0$
  - $P_i = x_i H_i$
  - H_i is Henry’s Law constant
  - $H_i = f(T)$
  - Tables available, but not in our book

Table 1: Some forms of Henry's law and constants (gases in water at 298 K), derived from [4]

equation:	$k_{H,pc} = \frac{p}{c}$	$k_{H,cp} = \frac{c}{p}$	$k_{H,px} = \frac{p}{x}$	$k_{H,cc} = \frac{c_{aq}}{c_{gas}}$
units:	$\frac{L \cdot atm}{mol}$	$\frac{mol}{L \cdot atm}$	atm	*dimensionless*
O_2	769.23	1.3×10^{-3}	4.259×10^{4}	3.180×10^{-2}
H_2	1282.05	7.8×10^{-4}	7.099×10^{4}	1.907×10^{-2}
CO_2	29.41	3.4×10^{-2}	0.163×10^{4}	0.8317
N_2	1639.34	6.1×10^{-4}	9.077×10^{4}	1.492×10^{-2}
He	2702.7	3.7×10^{-4}	14.97×10^{4}	9.051×10^{-3}
Ne	2222.22	4.5×10^{-4}	12.30×10^{4}	1.101×10^{-2}
Ar	714.28	1.4×10^{-3}	3.955×10^{4}	3.425×10^{-2}
CO	1052.63	9.5×10^{-4}	5.828×10^{4}	2.324×10^{-2}

where:

c = amount concentration of gas in solution (in mol/L)
p = partial pressure of gas above the solution (in atm)
x = mole fraction of gas in solution (dimensionless)

(from Wikipedia)

Henry’s Law

(in place of Raoult’s Law)

Find the equilibrium mole fraction of O_2 in water if air above water is at 298 K

- $k_{H,px,O2} = 4.259e4$ atm
- $P_{O2} = x_{O2}\, k_{H,px,O2}$
- But $P_{O2} = 0.21$ atm
- $x_{O2} = P_{O2}/k_{H,px,O2}$
- So $x_{O2} = .21 \text{ atm}/4.259e4 \text{ atm}$

Mole fraction of O_2 in water = 4.9e-6, or 4.6 parts per million (ppm)

Table 1: Some forms of Henry's law and constants (gases in water at 298 K), derived from [4]

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where:

c = amount concentration of gas in solution (in mol/L)
p = partial pressure of gas above the solution (in atm)
x = mole fraction of gas in solution (dimensionless)

(from Wikipedia)

Terms you should know

- **VLE**
  - Vapor-liquid equilibrium
- **Bubble point calculation**
  - Any VLE calculation where x_i is known
  - T or P known, find y_i and P or T
- **Dew point calculation**
  - Any VLE calculation where y_i is known
  - T or P known, find x_i and P or T
- **Flash calculation**
  - VLE calculation where feed composition (z_i) is known along with T and P_{tot} of output
  - Need to find x_i's, y_i's, and L and V

Think….

- A closed vessel has a mixture of 50% benzene and 50% toluene
  - $T_{b,\ benzene}$ = 80.1°C
  - $T_{b,\ toluene}$ = 110.62°C

These T_b's are at 1 atm

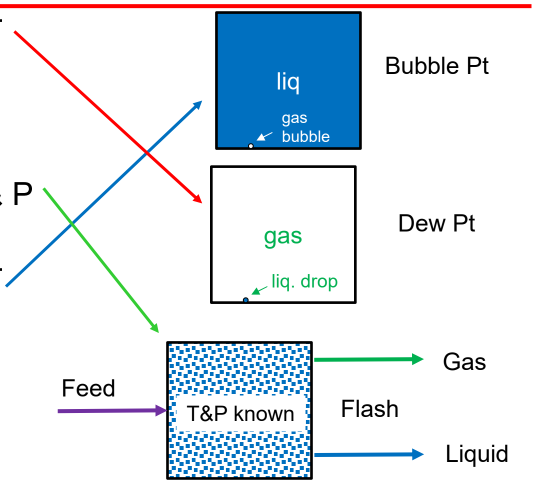
- Suppose you have this mixture at 1 atm and 25°C
  - What phases are present? All liquid since T < T_{boil} for both species
  - If you start heating the mixture, at what T will you start to get gas (assuming P stays constant)? 80.1°C
  - What will be the composition of the initial gas? 100% benzene
  - How will the gas composition change as you continue to heat the mixture? More and more toluene will vaporize
  - If the mixture is heated to 111°C, what will be the composition of the gas phase? 50% benzene and 50% toluene, just like initial liquid composition
  - What if you had a blanket of N_2 above the liquid?

N_2 could "suck up" benzene and toluene at T's below the boiling point based on P*'s

Matching

(2 + species, VLE)

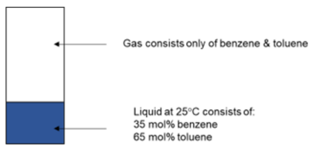
- y_i specified along with T or P
- Feed composition (z_i) specified along with T & P
- x_i specified along with T or P



Handouts

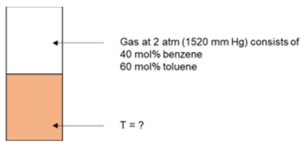
- Bubble pt calculation

Find: P_{tot}, y_B, y_T

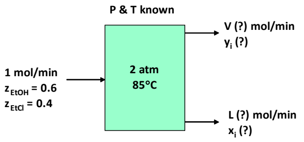


- Dew pt calculation

Find: T, x_B, x_T



- Flash calculation



Summary of Multicomponent Vapor-Liquid Equilibrium (VLE)

- x_i known (bubble point calculation)
  - If P_{tot} given, guess T to satisfy $P_{tot} = \Sigma P_i = \Sigma x_i P_i^*$
  - If T given, get $P_{tot} = \Sigma x_i P_i^*$
  - Then $y_i = x_i P_i^*/P_{tot}$

Note: this only works
If there is no non-condensable
gas above the liquid.

- y_i known (dew point calculation)
  - Use relation: $\Sigma x_i = 1$
  - If P_{tot} given, guess T to satisfy $\sum \frac{y_i P_{tot}}{P_i^*} = 1$
  - If T given, get $P_{tot} = \frac{1}{\sum \frac{y_i}{P_i^*}}$
  - Then $y_i = x_i P_i^*/P_{tot}$

Write in book!
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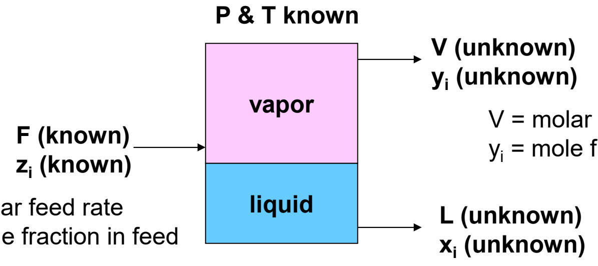
Flash Calculation



P & T known

vapor

liquid

F (known)
z_i (known)

V (unknown)
y_i (unknown)

L (unknown)
x_i (unknown)

F = molar feed rate
z_i = mole fraction in feed

V = molar flow rate of vapor
y_i = mole fraction in vapor

L = molar flow rate of liquid
x_i = mole fraction in liquid

Unknowns:	
V, L	2
y_i's	n-1
x_i's	n-1
Total	**2n**

Equations:	
$x_i P_i^* = y_i P_{tot}$	n
Species balances	n
Total	**2n**

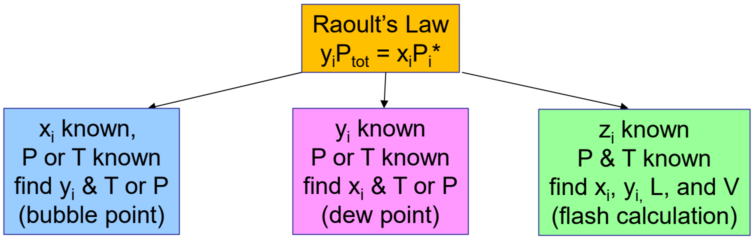
(Only n-1 x_i's because $\Sigma x_i = 1$)

Alternate: P known and y_i known

Flash Calculation

- z_i's known, 2 species, P&T known
  - Raoult's law for each species
    - $y_1P_{tot} = x_1P_1^*$
    - $(1-y_1)P_{tot} = (1-x_1)P_2^*$
    - Add these equations to get: $P_{tot} = x_1P_1^* + (1-x_1)P_2^*$
    - Solve for x_1
    - Get $y_1 = x_1P_1^*/P_{tot}$
  - Mole balances
    - $F = V + L$
    - $z_1F = y_1V + x_1L$
    - 2 equations, 2 unknowns (V & L)
- z_i's known, multiple species ➔ Solver

Multicomponent Logic Chart



Raoult's Law
$y_iP_{tot} = x_iP_i^*$

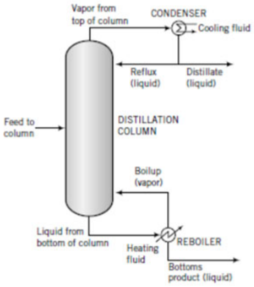
x_i known,
P or T known
find y_i & T or P
(bubble point)

y_i known
P or T known
find x_i & T or P
(dew point)

z_i known
P & T known
find x_i, y_i, L, and V
(flash calculation)

Hint on Prob 18.1

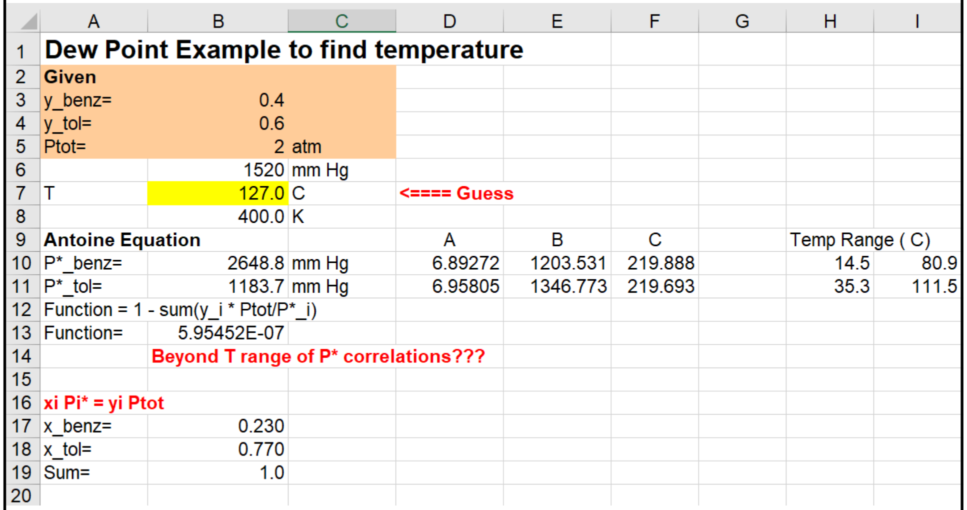
(b) Find T of vapor leaving top of column



Note that there is a tray near the top of the column that has liquid in equilibrium with the vapor leaving the column. This becomes a dew point problem since you know the vapor composition. The unknown is the temperature, which determines the vapor pressure of each species (just like the problem we did in class --- see next slide).

(c) Find T of reboiler

Since you calculated the composition of the bottoms product stream, which is a liquid, this is a bubble point problem to find the temperature (similar to part b except for a bubble point)



	A	B	C	D	E	F	G	H	I
1	**Dew Point Example to find temperature**								
2	**Given**								
3	y_benz=	0.4							
4	y_tol=	0.6							
5	Ptot=	2	atm						
6		1520	mm Hg						
7	T	127.0	C	**<==== Guess**					
8		400.0	K						
9	**Antoine Equation**			A	B	C		Temp Range (C)	
10	P*_benz=	2648.8	mm Hg	6.89272	1203.531	219.888		14.5	80.9
11	P*_tol=	1183.7	mm Hg	6.95805	1346.773	219.693		35.3	111.5
12	Function = 1 - sum(y_i * Ptot/P*_i)								
13	Function=	5.95452E-07							
14		**Beyond T range of P* correlations???**							
15									
16	**xi Pi* = yi Ptot**								
17	x_benz=	0.230							
18	x_tol=	0.770							
19	Sum=	1.0							
20									

Extra Notes

Bubble Point, or if x_i's known

- x_i's known, y_i's wanted (n unknowns)
- P or T given, T or P wanted <u>(1 unknown)</u>

Total unknowns: n+1

<u>Equations</u>

- $x_i P_i^* = y_i P_{tot}$ (n eqns)
- $\Sigma y_i = 1$ (1 eqn)

- Strategy: Solve for y_i, then sum all equations to eliminate the unknown y_i because $\Sigma y_i = 1$

$$y_i = x_i P_i^*/P_{tot}$$

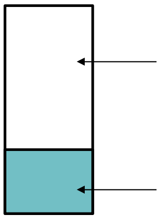
Summing both sides,

$$\Sigma y_i = 1 = \Sigma(x_i P_i^*/P_{tot})$$

- If T known, calculate P_i^*'s, solve for P_{tot}, then use Raoult's law to get y_i's
- If P_{tot} known, guess T, find P_i^*'s, see if $\Sigma(x_i P_i^*/P_{tot}) = 1$
  - ITERATE

“Bubble Point” Example

Find: P_{tot}, y_B, y_T



Gas consists only of benzene & toluene

Liquid at 25°C consists of:
40 mol% benzene
60 mol% toluene

Dew Point, or if y_i’s known

- y_i’s known, x_i’s wanted (n unknowns)
- P or T given, T or P wanted (1 unknown)

Total unknowns: n+1

Equations

- $x_i P_i^* = y_i P_{tot}$ (n eqns)
- $\Sigma x_i = 1$ (1 eqn)

- Strategy: Solve for x_i, then sum all equations to eliminate the unknown x_i because $\Sigma x_i = 1$

$$x_i = (y_i * P_{tot}/P_i^*)$$

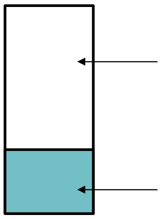
Summing both sides,

$$\Sigma x_i = 1 = P_{tot}\Sigma(y_i / P_i^*)$$

- If T known, solve for P_{tot}, then use Raoult’s law to get x_i’s
- If P_{tot} known, guess T, find P_i^*’s, see if $P_{tot}\Sigma(y_i / P_i^*) = 1$
  - ITERATE

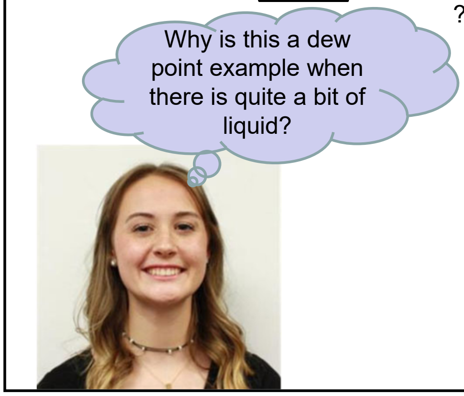
“Dew Point” Example

Find: T, x_B, x_T

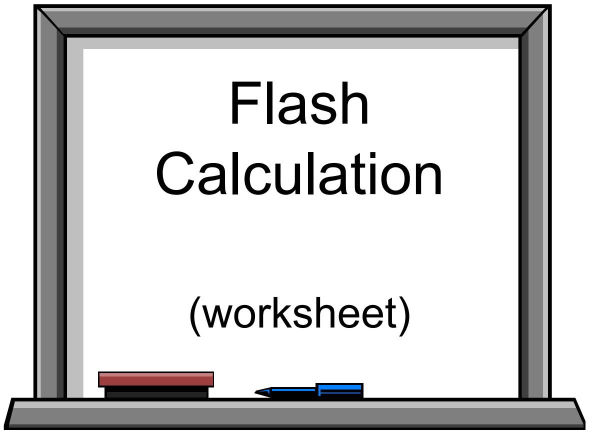


Gas at 2 atm (1520 mm Hg) consists of
40 mol% benzene
60 mol% toluene

Liquid consists of:
? mol% benzene
? mol% toluene



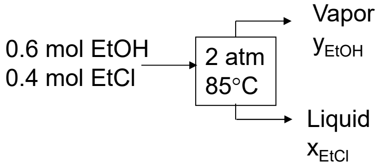
Why is this a dew point example when there is quite a bit of liquid?



Flash Calculation

(worksheet)

Sample Flash Calculation



At 85°C, P^*_{EtOH} = 985.1 mm Hg
P^*_{EtCl} = 6362.5 mm Hg

P_{tot} = 1520 mm Hg

Find L, V, y_i's, x_is

Mole Balance: $1 = V + L$
EtOH Balance: $0.6 = y_{EtOH}V + x_{EtOH} L$

Raoult's Law:

$$\begin{array}{r} y_{EtOH} P = x_{EtOH}P^*_{EtOH} \\ (1-y_{EtOH}) P = (1-x_{EtOH})P^*_{EtCl} \\ \hline P = x_{EtOH}P^*_{EtOH} + (1-x_{EtOH})P^*_{EtCl} \end{array}$$

Add these two equations

Solve for x $x_{EtOH} = \frac{P - P^*_{EtCl}}{P^*_{EtOH} - P^*_{EtCl}} = \frac{1520 - 6362.5}{985.1 - 6362.5} = 0.9$ so $x_{EtCl} = 0.1$

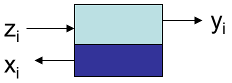
Using Raoult's law: $y_{EtOH}(1520) = (0.9)(985.1)$ so $y_{EtOH} = 0.583$
$y_{EtCl} = 0.417$

Now use mole balances: $1 = V + L$
$0.6 = 0.583V + 0.9L$

2 eqns, 2 unknowns: $L = 0.0536$
$V = 0.9464$

Hint on 18.2
(replaced in 2021)

A. Partial condenser



- However, at minimum pressure, $m_{liq} \to 0$, so y_i is known ($= z_i$)
- If y_i is known, this is a dew point calculation!
  - T known, find P!

B. Total condenser

- However, at minimum pressure, $m_{vap} \to 0$, so x_i is known ($= z_i$)
- If x_i is known, this is a bubble point calculation!
  - T known, find P!