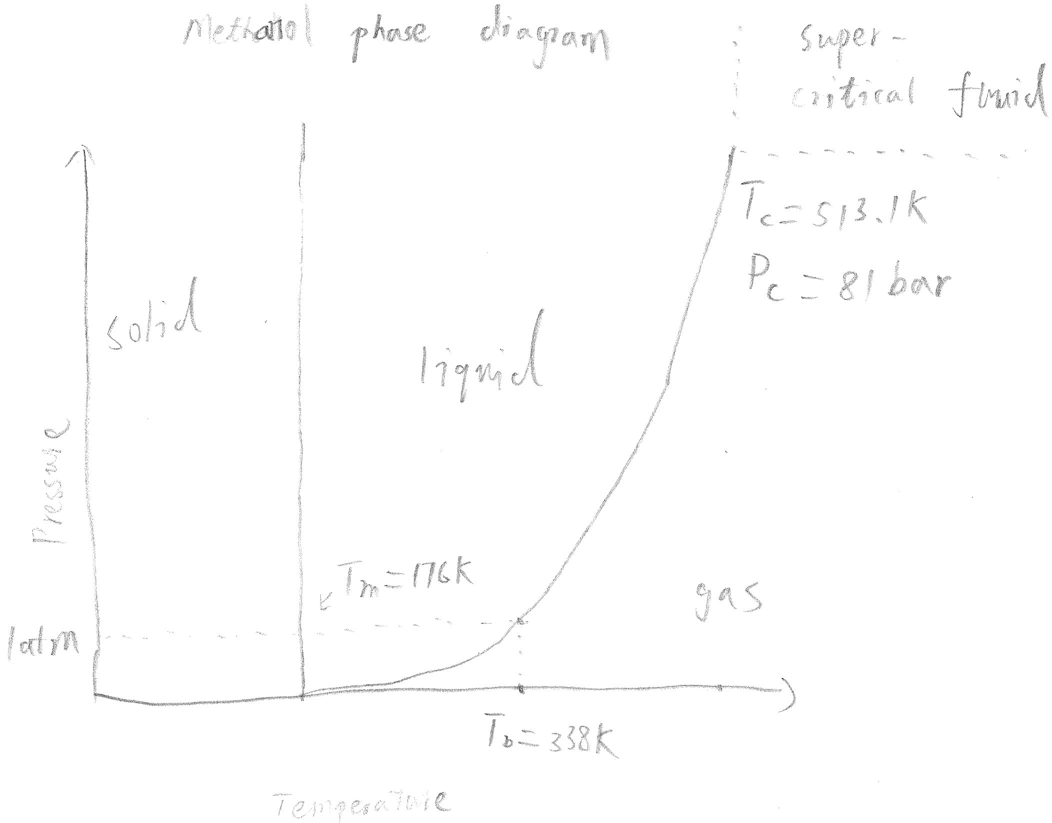
CBE 20255
HW6

1\. Methanol phase diagram

1)



2) The melting temperature of methanol goes up with increasing pressure.

3) We can estimate the pressure using Clausius–Clapeyron equation:

$$\ln\left(\frac{P_2}{P_1}\right) = \frac{\Delta H}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

As we already have 2 sets of P, T

$$\begin{cases} P = 1atm \\ T_b = 338K \end{cases} \qquad \begin{cases} P_c = 81\,bar \\ T_c = 513.1K \end{cases}$$

We can there-for solve for ΔH

$$\ln\left(\frac{81\ bar}{1\,atm}\right) = \frac{\Delta H}{R}\left(\frac{1}{338K} - \frac{1}{513.1K}\right)$$

$$\longrightarrow \Delta H = 36.1\ kJ/mol$$

We know $T_3 = 100°C = 373.15K$

$$\ln\left(\frac{P_2}{P_3}\right) = \frac{\Delta H}{R}\left(\frac{1}{T_3} - \frac{1}{T_2}\right)$$

$$P_3 = P_2 / \exp\left(\frac{\Delta H}{R}\left(\frac{1}{T_3} - \frac{1}{T_2}\right)\right)$$

$$= 1\,atm / \exp\left(\frac{36.1\ kJ/mol}{8.314\times10^{-3}\ kJ/mol\cdot k}\left(\frac{1}{373.15K} - \frac{1}{338K}\right)\right)$$

$$= 3.35\ atm$$

4) Antoin Equation:

$$\log_{10}(P) = A - B/(T+C)$$

P = vapor pressure (bar)

T = temperature

For methanol, $A = 5.15853$, $B = 5.20409$, $C = 5.31301$ from Nist Webbook

$T = 373.15K$

So $P = 10^{[A - B/(T+C)]}$

$$= 10^{5.15853 - \frac{1569.613}{-34.846 + 373.15}}$$

$$= 3.302 \text{ bar}$$

5) If $P = (1+1.5)\,atm = 2.5\,atm$

$$\log_{10} P = A - B/(T+C)$$

$$T = \frac{B}{A - \log_{10} P} - C$$

$$= \frac{1569.613}{5.15853 - \log_{10}(2.5 \times 1.01\,bar)} + 34.846$$

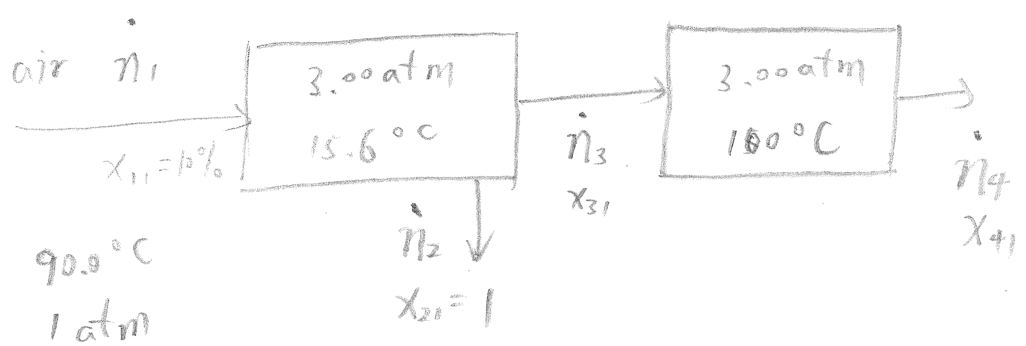
$$= 364.9\,K < 373.15\,K$$

So the vapor is superheated by 8.3 degree.

6) The due pressure at $100°C$ equals to the vapor pressure at $100°C$, which is 3.302 bar

2. $1 = H_2O$

1)



At $3.00\,atm$ and $15.6°C$,

$$P^{sat}_{H_2O} = 1773\,Pa$$

So in stream 3, $P_{H_2O} = 1773\,Pa$

$$x_{31} = \frac{P_{H_2O}}{P_{total}} = \frac{1773\,Pa}{3\,atm} \cdot \frac{atm}{101325\,Pa} = 0.58\%$$

Assume $\dot{n}_1 = 100\,mol/s$

$$\begin{cases} \dot{n}_1 = \dot{n}_2 + \dot{n}_3 \\ \dot{n}_1 x_{11} - \dot{n}_2 = \dot{n}_3 x_{31} \end{cases}$$

$$100 = \dot{n}_2 + \dot{n}_3$$
$$100 \cdot 10\% - \dot{n}_2 = 0.58\%\, \dot{n}_3$$

So $\begin{cases} \dot{n}_2 = 9.5\,mol/s \\ \dot{n}_3 = 90.5\,mol/s \end{cases}$

Fraction of water condensed $= \dfrac{\dot{n}_2}{\dot{n}_1 x_{11}} = \dfrac{9.5}{10} = 95\%$

2)

Relative humidity = ϕ

$$= \frac{P_{H_2O}}{P^*_{H_2O}}$$

P_{H_2O} = partial pressure of H_2O at 100°C

$P^*_{H_2O}$ = Vapor pressure of H_2O at 100°C

$P_{H_2O} = 1773\,Pa$ from part (1)

$P^*_{H_2O} = 102231\,Pa$

So $\phi = \frac{1773\,Pa}{102231\,Pa} = 1.73\,\%$

3) Ideal gas law:

$$P\dot{V} = \dot{n}RT$$

$$\frac{\dot{V}_1}{\dot{V}_4} = \frac{\dot{n}_1 RT_1/P_1}{\dot{n}_4 RT_4/P_4} = \frac{100\,mol/s \cdot 363.15K/1\,atm}{90.5\,mol/s \cdot 473.15K/3\,atm}$$

$$= 2.544$$

So $\frac{\text{Outlet}}{\text{Inlet}} = \frac{\dot{V}_4}{\dot{V}_1} = 0.393$

3. 1 = propane 2 = n-butane 3 = iso-butane

1) At 20°C, $P_i^*(293.15K) = 10^{A-\frac{B}{T+C}}$

$P_1^* = 8.377$ bar

$P_2^* = 2.075$ bar

$P_3^* = 3.008$ bar

Antoine parameters used are shown in part (3)

According to Raoult's Law,

$P_i = P_i^* \cdot x_i$

So $P = 8.377\text{bar} \cdot 50\% + 2.075\text{ bar} \cdot 30\%$

$+ 3.008\text{ bar} \cdot 20\% = 5.413\text{ bar}$

2) $y_i = \frac{P_i}{P}$

So
$$\begin{cases} y_1 = \frac{8.377 \cdot 50\%}{5.413} = 77.4\% \\ y_2 = \frac{2.075 \cdot 30\%}{5.413} = 11.5\% \\ y_3 = \frac{3.008 \cdot 20\%}{5.413} = 11.1\% \end{cases}$$

3) $P_{total} = P_1 + P_2 + P_3$

$P_1 = 10^{A - \frac{B}{T+C}} X_1$

$A = 4.53678$

$B = 1149.36$

$C = 24.906$

$P_2 = 10^{A - \frac{B}{T+C}} X_2$

$A = 4.35576$

$B = 1175.581$

$C = -2.071$

$P_3 = 10^{A - \frac{B}{T+C}} X_3$

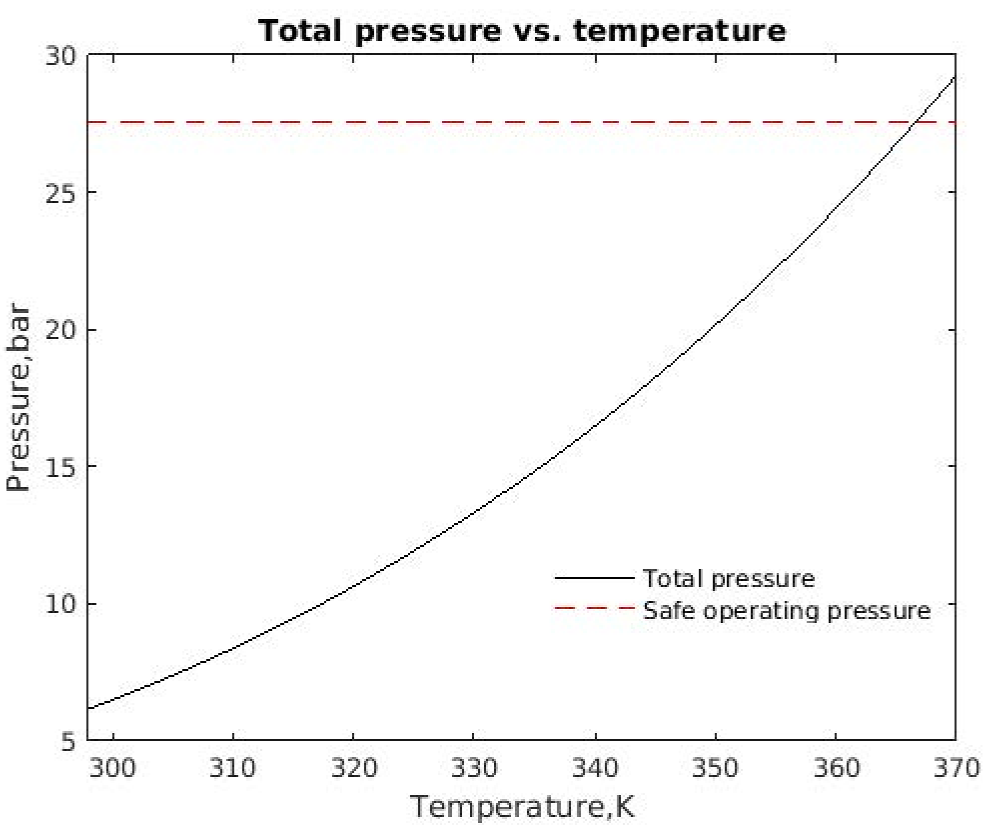
$A = 4.3281$

$B = 1132.108$

$C = 0.918$

A, B, C values are from Nist Webbook.

P_{tot} is a function of T.



When T>366.7 K, total pressure exceeds the safe operating pressure

4) According to Gibbs phase rule,

$$F = C - P + 2$$

If solids of all 3 components are in equilibrium with liquid,

$C = 3$ $\quad$ $P = \underbrace{3}_{\text{solid}} + \underbrace{1}_{\text{liquid mixture}} = 4$

$$F = 3 - 4 + 2 = 1$$

You still have a degree of freedom, so it is likely to have 3 solids - liquid equilibrium.

4.

1) At bubble point,

$$P = \sum_i x_i P_i^*(T)$$

y_i = vapor composition of i

x_i = liquid composition of i

$P_i^*(T)$ = vapor pressure of i

P = Total pressure of gas

1 = n-pentane   2 = iso-pentane

At 120 °C

$$\begin{cases} A = 3.9892 \\ B = 1070.617 \\ C = -40.454 \\ P_1^* = 10^{A-\frac{B}{T+C}} = 8.988\ \text{bar} \end{cases}$$

From Nist Webbook

$$\begin{cases} A = 3.9718 \\ B = 1021.864 \\ C = -43.231 \\ P_2^* = 10^{A-\frac{B}{T+C}} = 11.260\ \text{bar} \end{cases}$$

From Nist Webbook

$$8.988 \times 0.5 + 11.260 \times 0.5 = P$$

So $P = 10.124$ bar

$$y_1 = \frac{8.988}{8.988 + 11.260} = 44.4\%$$

$$y_2 = \frac{11.260}{8.988 + 11.260} = 55.6\%$$

2) At dew point,

$\sum x_i = 1$

$x_i = y_i P / p_i^*(T)$

So $0.5 / \frac{8.988}{P} + 0.5 / \frac{11.260}{P} = 1$

$P = 9.997$ bar

$x_1 = 0.5 / \frac{8.988}{9.997} = 55.6\%$

$x_2 = 0.5 / \frac{11.260}{9.997} = 44.4\%$

3) $P = 2.5$ atm

At bubble point,

$P = \sum_i x_i P_i^*(T)$

$\rightarrow \quad 0.5 P_1^*(T) + 0.5 P_2^*(T) = P = 2.5 \text{ atm} \quad ①$

$P_1^* = 10^{A - \frac{B}{C+T}} \qquad P_2^* = 10^{A - \frac{B}{T+C}}$

Antoine paramters used are the same as in part (1).

T can be solved for using equation ①.

Matlab code for solving the equation is attached in the end of solution.

$T = 333.9 \text{ K}$

$$y_1 = \frac{0.5 P_1^*}{0.5 P_1^* + 0.5 P_2^*} = 43.4\%$$

$$y_2 = \frac{0.5 P_2^*}{0.5 P_1^* + 0.5 P_2^*} = 56.6\%$$

4) $P = 2.5\,atm$

At dew point,

$$\sum x_i = 1$$

$$x_i = y_i P / p_i^*(T)$$

$$p_1^*(T) = 10^{A - \frac{B}{T+C}}$$

Antoine parameters used are the same as in part (1)

So $$\frac{0.5 \cdot 2.5\,atm}{p_1^*(T)} + \frac{0.5 \cdot 2.5\,atm}{p_2^*(T)} = 1 \quad (2)$$

Using Matlab (code attached in the end),

T can be solved for using equation (2)

$$T = 334.5\,K$$

$$x_1 = \frac{0.5}{p_1/2.5\,atm} = 56.6\%$$

$$x_2 = \frac{0.5}{p_2/2.5\,atm} = 43.4\%$$

Matlab script

Problem 4

3)

```
clear all
syms T
vpasolve(10^(3.9892-1070.617/(-40.454+T))+10^(3.9718-1021.864/(-43.231+T))...
  == 5.05,T,[100 500])
```

4)

```
clear all
syms T
vpasolve(0.5*2.5*1.01/10^(3.9892-1070.617/(-40.454+T))+...
  0.5*2.5*1.01/10^(3.9718-1021.864/(-43.231+T))...
  == 1,T,[100 500])
```

syms T is to define your variable in the equation.

vpasolve(equantion,variable,range of variable) is to solve the equation numerically for variable in the defined range.