Midterm 2017W solution 1+2

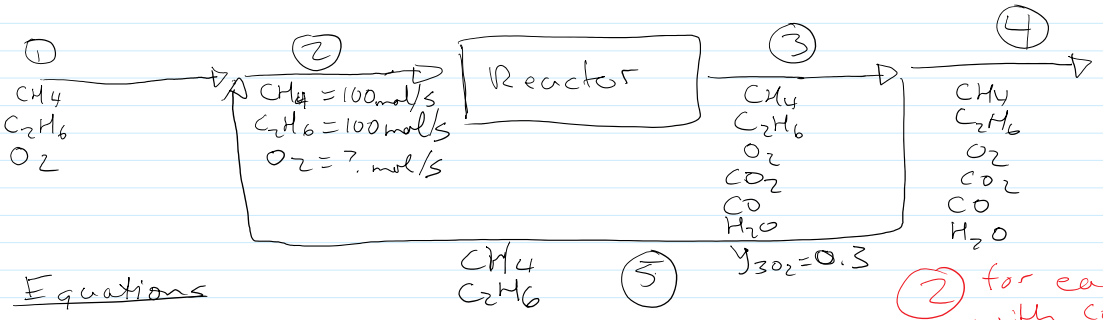
November 9, 2017 1:33 PM

1. (40 points) An unknown quantity of methane, ethane and oxygen are being fed into a process. They are fed at such a rate so as to ensure that after mixing with a recycle stream an equimolar mixture of methane (CH_4) and ethane (C_2H_6) is fed to a reactor at a rate of 200 mol/s. Oxygen is not contained in the recycle stream, but the amount fed into the process and therefore the reactor isin excess of what is required. Combustion takes place in the reactor. The single pass conversion of methane is 80% and the single pass conversion of ethane is 70%. The gas leaving the reactor contains 30 mole% O_2. This gas is sent to a separator where all the reaction products and 10% of the methane and ethane in the entering stream are sent out of the system as exhaust. The remaining methane and ethane form the recycle stream. In the reactor, for every 5 mol of CO produced, 95 mol of CO_2 are produced.

a. Draw a diagram for the system, listing the compounds present in each stream. (15 points)

b. Find the overall conversions of methane and ethane. (10 points)

c. Find the percent excess oxygen in the feed to the reactor (15 points)



Equations

Single Pass conversions

CH_4: $0.8 = \frac{n_{2CH_4} - n_{3CH_4}}{n_{2CH_4}}$ (1)

C_2H_6: $0.7 = \frac{n_{C_2H_6} - n_{3C_2H_6}}{n_{2C_2H_6}}$ (1)

(2) for each stream with correct species −1 if species missing

Gas separation (10% in stream 4 from stream 3)

$n_{4CH_4} = 0.1\, n_{3CH_4}$ (1) $\quad n_{4C_2H_6} = 0.1\, n_{3C_2H_6}$ (1)

Partial combustion

$\frac{n_{CO}}{n_{CO_2}} = \frac{5}{95}$ or $n_{CO_2} = 19\, n_{CO}$ (1)

b) Solving for overall conversion

From single pass conversions:

$n_{3CH_4} = n_{2CH_4}(1 - 0.8) = 20$ mol/s (1)

$n_{3C_2H_6} = n_{2C_2H_6}(1 - 0.7) = 30$ mol/s (1)

From gas separation equations

$n_{4CH_4} = 0.1 \times n_{3CH_4} = 2$ mol/s (1)

$n_{4C_2H_6} = 0.1 \times n_{3C_2H_6} = 3$ mol/s (1)

From balance on separator after reactor

$n_{5CH_4} = n_{3CH_4} - n_{4CH_4} = 18$ mol/s (1)

$n_{5C_2H_6} = n_{3C_2H_6} - n_{4C_2H_6} = 27$ mol/s (1)

From balance on mixing point before reactor

$n_{1CH4} = n_{2CH4} - n_{5CH4} = 82 \text{ mol/s}$ (1)

$n_{1C2H6} = n_{2C2H6} - n_{5C2H6} = 73 \text{ mol/s}$ (1)

Overall conversions

CH_4 : $\frac{n_{CH4\,in} - n_{CH4\,out}}{n_{CH4\,in}} = \frac{82 - 2}{82} = 0.976$ or 97.6% (1)

C_2H_6 : $\frac{n_{C2H6\,in} - n_{C2H6\,out}}{n_{C2H6\,in}} = \frac{73 - 3}{73} = 0.959$ or 95.9% (1)

c) Using atomic balances on reactor (Note ξ can be used, but it is very difficult due to CO_2/CO reaction ratio)

Atomic balance on C: IN = OUT

$$n_{2CH4} \cdot 1\frac{\text{mol C}}{\text{mol CH4}} + n_{2C2H6} \cdot 2\frac{\text{mol C}}{\text{mol C2H6}} = n_{3CH4} \cdot 1 + n_{3C2H6} \cdot 2 + n_{3CO} + n_{3CO2}$$

Use $n_{3CO2} = 19\, n_{3CO}$

$$100 \cdot 1 + 100 \cdot 2 = 20 \cdot 1 + 30 \cdot 2 + n_{3CO} + 19 n_{3CO}$$

$$300 = 80 + 20 n_{3CO}$$

$n_{3CO} = 11 \text{ mol/s}$ (2)

$n_{3CO2} = 19 \times n_{3CO} = 209 \text{ mol/s}$ (2)

H Balance: IN = OUT

$$100 \cdot 4 + 100 \cdot 6 = 20 \cdot 4 + 30 \cdot 6 + n_{3H2O} \cdot 2$$

$$n_{3H2O} = \frac{1000 - 80 - 180}{2} = 370 \text{ mol/s}$$ (2)

Now using known O_2 fraction

$$y_{3O2} = 0.3 = \frac{n_{3O}}{n_{3\,tot}} = \frac{n_{3O2}}{n_{3CH4} + n_{3C2H6} + n_{3CO} + n_{3CO2} + n_{3O2} + n_{3H2O}}$$

$$0.3(n_{3CH4} + n_{3C2H6} + n_{3CO2} + n_{3CO} + n_{3H2O}) + 0.3\, n_{3O2} = n_{3O2}$$

$$0.3(20 + 30 + 209 + 11 + 370) = 0.7\, n_{3O2}$$

$n_{3O2} = 274.3 \text{ mol/s}$ (2)

O2 balance IN = OUT

$$2 \cdot n_{2O2} = 2 \cdot n_{3O2} + 2 n_{3CO2} + n_{3CO} + n_{3H2O}$$

$$n_{2O2} = \frac{2 \cdot (274.3) + 2 \cdot 209 + 11 + 370}{2}$$

$n_{2O2} = 673.8 \text{ mol/s}$ (2)

n_{O2} theoretical determination

n_O2 theoretical determination

2 reactions, theoretical = complete combustion

① $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

② $C_2H_6 + 3.5O_2 \rightarrow 2CO_2 + 3H_2O$

So # moles according to equations above:

reaction ① $2 \times 100 = 200$ mol/s (2)

reaction ② $3.5 \times 100 = 350$ mol/s (2)

$n_{theo} = 550$ mol/s

$$\%\text{ excess} = \frac{n_{actual} - n_{theo}}{n_{theo}} = \frac{637.8 - 550}{550} = 0.225 \text{ or } 22.5\%$$ (1)

2. (30 points) A liquid stream at a temperature of 60 °C and a pressure of 21 bar contains equimolar amounts of two chemically similar components A and B (ie. an ideal solution). A has a molecular weight of 60 g/mol and B has a molecular weight of 70 g/mol. In a steady-state flow process, the stream undergoes a decrease in pressure to 1.0 bar at a constant temperature of 60°C. This mixture is then allowed to equilibrate and a vapour and liquid stream exit the process. The vapour stream exits the process flows at a molar flow rate equal to 60% of the molar flow rate of the entering liquid. The rest of the fluid exits the process as a liquid. The vapor pressure of component A is known to be 0.74 bar at 60 °C.

a. Draw a block diagram to represent this process, labelling known and unknown quantities. Using the Gibb's phase rule is the equilibrated mixture in the process is fully thermodynamically specified? Why or why not? (10 points)

b. What is the molar composition of the vapor stream and liquid streams exiting the process? (8 points)

c. What is the vapor pressure of component B? Note that if you cannot find the compositions from part a use the following compositions: liquid mole fraction of component B being 0.7, vapour mole fraction of component B being 0.3. You do not need to change these if you solve part b later (2 points)

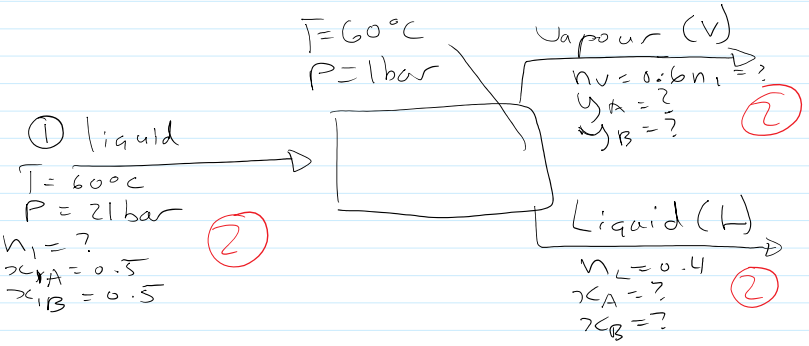
d. In a separate adsorption system 10 litres of a mixture containing only A and air at 40% relative saturation of A is put into contact with activated carbon. A is a pollutant and is adsorbed onto the carbon and the system pressure at 1 bar, and volume at 10 L, is held constant by pumping pure air into the system. The temperature remains at 60 °C throughout the process. The system follows the Langmuir isotherm below. If we want to significantly reduce the amount of A in the system down to to 5,000 parts per million by volume, what will be the amount of carbon required? (10 points)

$$X_i^* = \frac{aK_L'p_i}{1 + K_L'p_i}$$

$Where\ K_L' = 72.96\ bar^{-1}$

$$a = 0.794\ \frac{grams\ of\ A}{kg\ of\ activated\ carbon}$$

a)



(2) (2) (2)

Gibb's phase rule: $C - P + 2 = 2(A,B) - 2(V,L) + 2 = 2$ (2)

Need 2 intrinsic variables, these are T = 60°C and P = 1 bar

So fully specified thermodynamically (2)

b) Vapour composition, do material balance on A

① $n_1 x_{1A} = n_V y_A + n_L x_A$ (2)

combine with $y_A P = x_A P_A^*$ so $y_A = \frac{x_A P_A^*}{P}$ (2)

$y_1 x_{1A} = 0.6 y_1 \frac{x_A P_A^*}{P} + 0.4 y_1 x_A$

$0.5 = x_A \left(0.6 \frac{P_A^*}{P} + 0.4\right)$

$x_A = \frac{0.5}{\left(0.6 \frac{0.74\,bar}{1\,bar} + 0.4\right)} = 0.59$ (1) $x_B = 1 - x_A = 0.41$ (1)

From (1) $y_A = \frac{0.5 - 0.4 x_A}{0.6} = 0.44$ (1) $y_B = 1 - y_A = 0.56$ (1)

c) $y_B P = x_B P_B^*$

$P_B^* = \frac{y_B P}{x_B} = \frac{0.56\,(1\,bar)}{0.41} = 1.36\,bar$ (2)

d) Need to find initial and final concentrations of A

$P_A^* = 0.74\,bar$, with 40% relative saturation, so

$P_A = 0.4 \times P_A^* = 0.4 \times 0.74 = 0.296\,bar$ (1)

initial mole frac $y_{A0} = \frac{P_A}{P} = \frac{0.296\,bar}{1\,bar} = 0.296$ (1)

final mole frac $y_{Af} = \frac{5}{1000} = 5 \times 10^{-3}$ or 0.005 (1) $P_{Af} = y_{Af} P = 5 \times 10^{-3}\,bar$ (1)

$X_A^* = \frac{a k_L' P_{Af}}{(1 + k_L' P_{Af})} = \frac{72.96 \times 0.794 \times 5 \times 10^{-3}}{(1 + 72.96 \times 5 \times 10^{-3})} = \frac{0.2896}{1.004}$

$X_A^* = 0.212\,g_A / kg\ Carbon$ (2)

Amount adsorbed $= n (y_{A0} - y_{Af})$

$n = \frac{PV}{RT} = \frac{1\,bar \cdot 10\,L}{\left(8.314 \times 10^{-2} \frac{mol \cdot K}{bar \cdot L}\right)(60 + 273.15)} = 0.3610\,moles$ (1)

$n_{ads} = 0.3610 (0.296 - 0.05) = 0.105\,moles$ (1)

$m_{ads} = n_{ads} \times MW_A = 0.105\,mol \times 60\,g/mol = 6.3\,g$ (1)

$m_C = \frac{m_{ads}}{X_A^*} = \frac{6.3\,g_A}{0.212\,g_A/kg\,carbon} = 29.7\,kg\ Carbon$ (1)

$m_C = 22$ kg Carbon