CBE 20255 HW4 solution

1. NO!

1. $4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O$

2. $4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O$

lb-mole 10 X

From stoichiometry,

$$\frac{10}{X} = \frac{4}{5} \longrightarrow X = 13$$

13 lb-mole of O_2 is required.

3. To completely react NH_3 at a flow rate of 100 kmol/hr, X kmol/hr of O_2 is required.

From stoichiometry,

$$\frac{100}{X} = \frac{4}{5} \longrightarrow X = 125 \text{ kmol/hr}$$

To maintain a 40% excess of O_2, O_2 flow rate is y kmol/hr.

$$\frac{y - X}{X} = 40\% \longrightarrow y = 180 \text{ kmol/hr}$$

So 180 kmol/hr of O_2 feed is required.

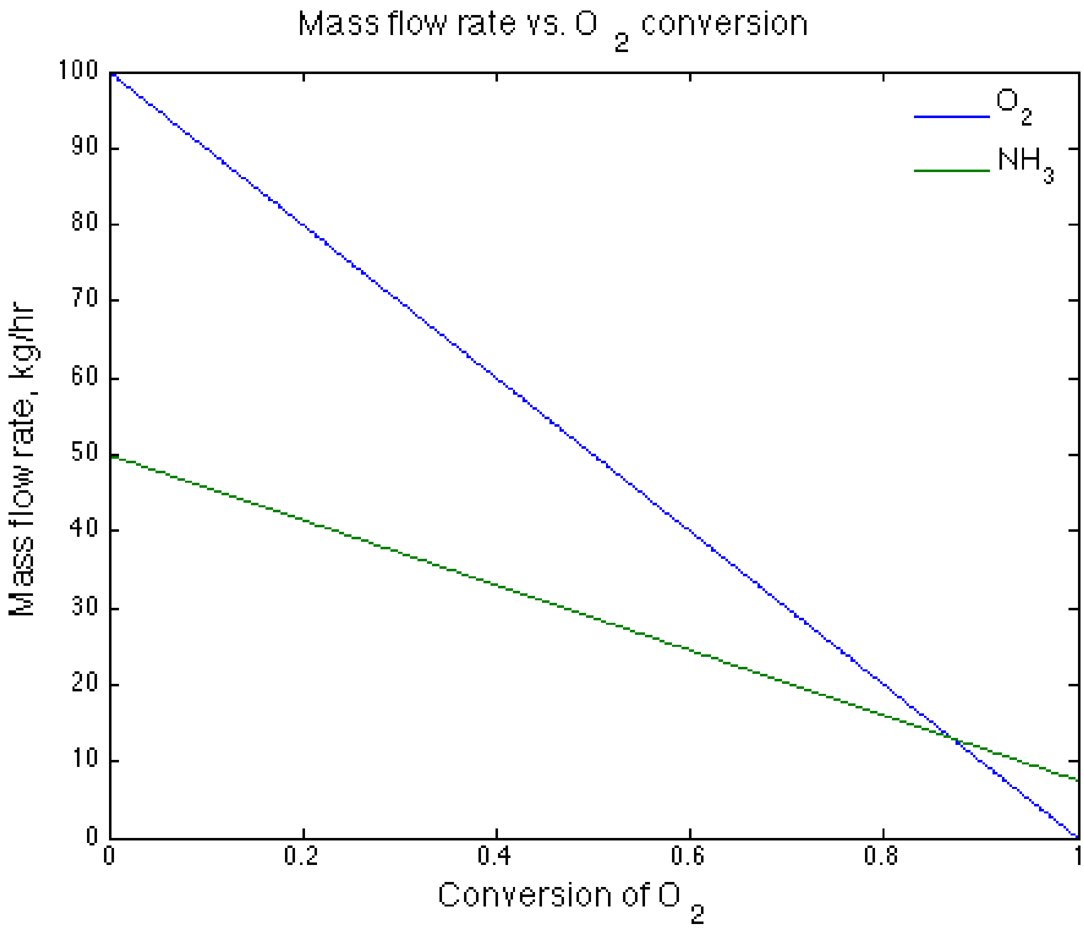
4. As $\frac{50.0 \text{ kg/hr } NH_3}{100.0 \text{ kg/hr } O_2} > \frac{4 \times 17}{5 \times 32}$, O_2 is limiting reactant.

X is conversion of O_2

Outlet mass flow rate of O_2 = 100.0 kg/hr (1 − X)

Outlet mass flow rate of NH_3 = $50.0 \text{ kg/hr} - \frac{4 \cdot 100 X}{5 \, MW_{O_2}} MW_{NH_3}$

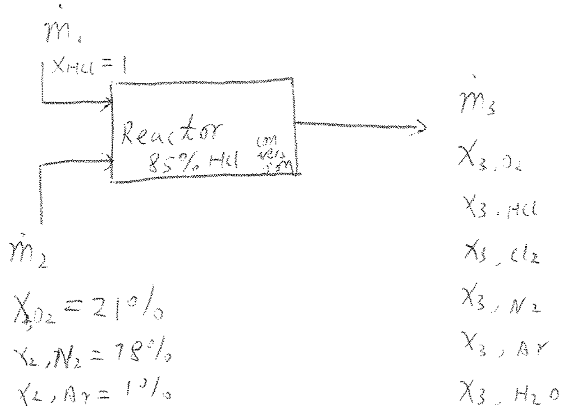
$$= 50.0 \text{ kg/hr} - \frac{85}{2} X$$


Mass flow rate vs. O 2 conversion
O2
NH3
Mass flow rate, kg/hr
Conversion of O 2
0
10
20
30
40
50
60
70
80
90
100
0
0.2
0.4
0.6
0.8
1

2. Deacon Blues (Or an Ode to Wake Forest) ☆

1. $4HCl + O_2 \longrightarrow 2Cl_2 + 2H_2O$

2.



3. Atomic balance

$$\begin{cases} H: & \dot{m}_1 X_{HCl} = \dot{m}_3 X_{3,HCl} + 2\dot{m}_3 X_{3,H_2O} \\ O: & 2\dot{m}_2 X_{2,O_2} = 2\dot{m}_3 X_{3,O_2} + \dot{m}_3 X_{3,H_2O} \\ Cl: & \dot{m}_1 X_{HCl} = \dot{m}_3 X_{3,HCl} + 2\dot{m}_3 X_{3,Cl_2} \end{cases}$$

$$N: \quad 2\dot{m}_2 X_{2,N_2} = 2\dot{m}_3 X_{3,N_2}$$

$$Ar: \quad \dot{m}_2 X_{2,Ar} = \dot{m}_3 X_{3,Ar}$$

Assume $\boxed{\dot{m}_1 = 100\ kmol/hr}$ as basis, O_2 in dry air is 35% excess, so

$$\dot{m}_2 X_{2,O_2} = \dot{m}_1 X_{1,HCl} \cdot \frac{1}{4} \cdot (1+35\%) \longrightarrow \boxed{\dot{m}_2 = 88.2\ kmol/hr}$$

From stoichometry, we know $\boxed{X_{3,Cl_2} = X_{3,H_2O}}$

85% conversion of HCl $\longrightarrow$ $\boxed{\dot{m}_1 (1-85\%) = \dot{m}_3 X_{3,HCl}}$

We have 3 balance equations and 3 unknowns

$$\begin{cases} \dot{m}_3 X_{3,HCl} = 15\ kmol/hr \\ \dot{m}_3 X_{3,O_2} = 12.5\ kmol/hr \\ \dot{m}_3 X_{3,Cl_2} = 42.5\ kmol/hr \\ \dot{m}_3 X_{3,H_2O} = \cancel{43\ km} \ 42.5\ kmol/hr \end{cases}$$

$\dot{m}_3 X_{3,N_2} = 68.8 \text{ kmol/hr}$

$\dot{m}_3 X_{3,Ar} = 0.9 \text{ kmol/hr}$

So $\dot{m}_3 = 182.2 \text{ kmol/hr}$

$$\begin{cases} X_{3,HCl} = 8.2\% \\ X_{3,O_2} = 6.9\% \\ X_{3,Cl_2} = 22.3\% \\ X_{3,H_2O} = 22.3\% \\ X_{3,N_2} = 37.8\% \\ X_{3,Ar} = 0.5\% \end{cases}$$

4. X = extent of reaction

$$X = \dot{m}_1 X_{1,HCl} \cdot 85\% = 85 \text{ kmol/hr}$$

$$\dot{m}_3 X_{3,HCl} = \dot{m}_1 - X = 15 \text{ kmol/hr}$$

$$\dot{m}_3 X_{3,Cl_2} = \frac{2}{4} X = 42.5 \text{ kmol/hr}$$

$$\dot{m}_3 X_{3,H_2O} = \frac{2}{4} X = 42.5 \text{ kmol/hr}$$

$$\dot{m}_3 X_{3,O_2} = \dot{m}_2 X_{2,O_2} - \frac{1}{4} X$$

$$= 33.75 - \frac{1}{4} \cdot 85 = 12.5 \text{ kmol/hr}$$

$\dot{m}_3 X_{3,N_2} = 68.8 \text{ kmol/hr}$ $\quad\quad$ $\dot{m}_3 X_{3,Ar} = 0.9 \text{ kmol/hr}$

So $\dot{m}_3 = \sum_i^N \dot{m}_3 X_{3,i} = 182.2 \text{ kmol/hr}$

$$\begin{cases} X_{3,HCl} = 8.2\% \\ X_{3,O_2} = 6.9\% \\ X_{3,Cl_2} = 22.3\% \\ X_{3,H_2O} = 22.3\% \\ X_{3,N_2} = 37.8\% \\ X_{3,Ar} = 0.5\% \end{cases}$$

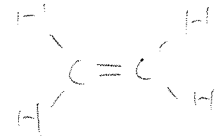
5.

Cost advantage: Pure O_2 reduces the total flowrate compared to dry air, which reduce the heat loss in heating up the irrelevant species in air.

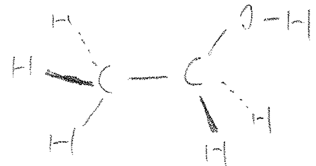
Cost disadvantage: Separating O_2 from air is an energy consuming process as the free energy is increased in such a process.

3. Commonly known as alcohol ☆

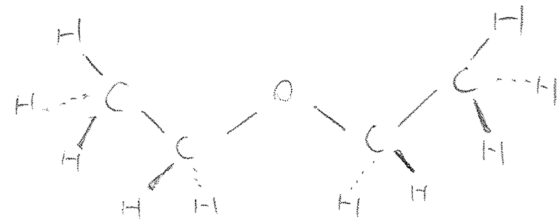
1. Ethylene :



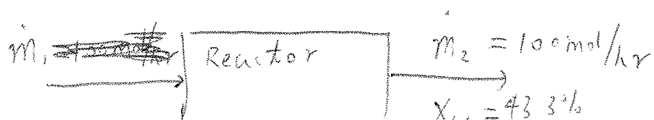
Ethanol :



Diethy ether :



2. 1 = ethylene   2 = steam   3 = inert   4 = ethanol   5 = ether



x_{11}
x_{12}
x_{13}

$C_2H_4 + H_2O \rightarrow C_2H_5OH$

$2C_2H_5OH \rightarrow (C_2H_5)_2O + H_2O$

$x_{21} = 43.3\%$
x_{22}
$x_{23} = 9.3\%$
$x_{24} = 2.5\%$
$x_{25} = 0.14\%$

3. 5 unknowns and 5 mole balance equations (ethylene, steam, inert, ethanol, ether)

0 DOF !

4. X_1 is the extent of reaction 1
X_2 is the extent of reaction 2

$$\begin{cases} \dot{m}_1 x_{13} = \dot{m}_2 x_{23} = 9.3\ mol/hr \\ \dot{m}_1 x_{11} - X_1 = \dot{m}_2 x_{21} = 43.3\ mol/hr \\ \dot{m}_1 x_{12} - X_1 + X_2 = 100\ mol/hr\,(1 - 43.3\% - 2.5\% - 0.14\% - 9.3\%) = 44.76\ mol/hr \\ X_2 = \dot{m}_2 x_{25} = 0.14\ mol/hr \\ X_1 - 2X_2 = \dot{m}_2 x_{24} = 2.5\ mol/hr \end{cases}$$

$$\rightarrow \begin{cases} X_1 = 2.75\ mol/hr \\ X_2 = 0.14\ mol/hr \\ x_{11} = 44.8\% \\ x_{12} = 46.1\% \end{cases}$$

$\dot{m}_1 = 103\ mol/hr$

5. Ethylene conversion

$$= \frac{\dot{m}_1 X_{11} - \dot{m}_2 X_{21}}{\dot{m}_1 X_{11}} = 5.9\%$$

6. Ethanol yield

$$= \frac{\dot{m}_2 X_{24}}{\dot{m}_1 X_{11}} = 5.4\%$$

7. Ethanol selectivity over ether

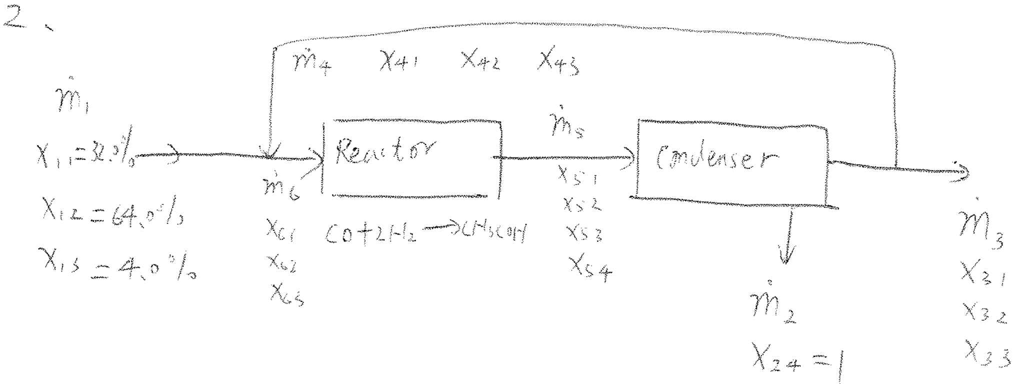
$$= \frac{\dot{m}_2 X_{24}}{\dot{m}_2 X_{25}} = 18$$

8. If the reactor was run to higher conversion, it should be expected (a) the ethanol yield will increase but (b) the selectivity will decrease.

4. Reduce, reuse, recycle ☆

1. $CO + 2H_2 \longrightarrow CH_3OH$

2. 1 = CO 2 = H_2 3 = N_2 4 = methanol



3.

$$\boxed{\begin{aligned} &\dot{m}_2 = 100\ \text{kmol/hr} \\ &\dot{m}_1 x_{11} - X = \dot{m}_3 x_{31} \\ &\dot{m}_1 x_{12} - 2X = \dot{m}_3 x_{32} \\ &X = \dot{m}_2 = 100\ \text{kmol/hr} \\ &\dot{m}_1 x_{13} = \dot{m}_3 x_{33} \end{aligned}}$$

X is the extent of overall reaction.

$x_{33} = x_{43}$ as they are from the same stream

$$\left.\begin{aligned} &\frac{\dot{m}_1}{\dot{m}_4} = \frac{1}{5} \qquad x_{63} = 13.0\% \\ &x_{13} = 4.0\% \end{aligned}\right\} \longrightarrow \dot{m}_6 x_{63} = \dot{m}_1 x_{13} + \dot{m}_4 x_{43}$$

$$\longrightarrow \boxed{\begin{aligned} x_{43} &= 14.8\% \\ &= x_{33} \end{aligned}}$$

From equations in boxes, we can solve

$$\begin{cases} x_{31} = 28.4\% \\ x_{32} = 56.8\% \\ \dot{m}_3 = 111\ \text{kmol/hr} \\ \dot{m}_1 = 411\ \text{kmol/hr} \end{cases}$$

4. Overall CO conversion

$$= \frac{\dot{m}_1 X_{11} - \dot{m}_3 X_{31}}{\dot{m}_1 X_{11}} = 76\%$$

5. Single pass CO conversion

$$= \frac{\dot{m}_6 X_{61} - \dot{m}_{51} X_{51}}{\dot{m}_6 X_{61}}$$

$$\dot{m}_6 X_{61} = \dot{m}_1 X_{11} + \dot{m}_4 X_{41}$$

$$= 411 \cdot 32.0\% + 411 \times 5 \times 28.4\%$$

$$= 715.14 \text{ kmol/hr}$$

$$\dot{m}_{51} X_{51} = \dot{m}_4 X_{41} + \dot{m}_3 X_{31}$$

$$= 615.144 \text{ kmol/hr}$$

So single pass CO conversion

$$= \frac{715.14 - 615.14}{715.14} = 14\%$$

6. (a) Recycle increases the overall conversion of the reactor.

(b) Purge avoid accumulation of inert and reactor blowup.

Atomic balance version of part 3, problem 4

3.

Atomic balance:

$$\boxed{\begin{aligned} &C: \quad \dot{m}_1 x_{11} = \dot{m}_3 x_{31} + \dot{m}_2 \\ &H: \quad 2\dot{m}_1 x_{12} = 2\dot{m}_3 x_{32} + \dot{m}_2 \\ &O: \quad \dot{m}_1 x_{11} = \dot{m}_3 x_{31} + \dot{m}_2 \\ &N: \quad 2\dot{m}_1 x_{13} = 2\dot{m}_3 x_{33} \end{aligned}}$$

$x_{33} = x_{43}$ as they are splitted from the same stream.

$$\left.\begin{aligned} &\frac{\dot{m}_1}{\dot{m}_4} = \frac{1}{5} \\ &x_{13} = 4.0\% \\ &x_{63} = 13.0\% \end{aligned}\right\} \quad \begin{aligned} &\dot{m}_6 x_{63} = \dot{m}_1 x_{13} + \dot{m}_4 x_{43} \\ &\rightarrow \boxed{x_{43} = x_{33} = 14.8\%} \end{aligned}$$

We have 3 independent equations and 3 unknowns. DOF=0

By solving the equations:

$$\left\{\begin{aligned} &\dot{m}_1 = 411 \text{ kmol/hr} \\ &\dot{m}_3 = 111 \text{ kmol/hr} \\ &x_{31} = 28.4\% \\ &x_{32} = 56.8\% \\ &x_{33} = 14.8\% \end{aligned}\right.$$