Department of Chemical Engineering
Thapar Institute of Engineering & Technology, Patiala

Course: Material and Energy Balances UCH301

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Material Balances with Chemical Reactions

- For writing balances on reacting components we include the consumption/generation terms in the general material balance equation:

$$\left(Flow\ of\ material\ \mathrm{in}\ \ through\ system\ boundaries\right)$$
$$-\left(Flow\ of\ material\ out\ \ through\ system\ boundaries\right)$$
$$+\left(Genration\ of\ material\ within\ the\ system\right)$$
$$-\left(Consumption\ of\ material\ within\ the\ system\right)$$
$$=\left(Accumulation\ of\ material\ within\ the\ system\right)$$

- Limiting/excess reactant is determined on the basis of feed i.e. We do not see what is happening in the reactor while determining limiting reactant, but amounts given in the feed are considered

Fractional conversion:

It is the ratio of the moles of reactant reacted to the moles of reactant fed.

Fractional conversional of reactant A:

f_A = moles of A reacted/ Moles of A fed

And, the fraction unreacted is equal to $1\text{-}f_A$.

Exercise

Acrylonitrile is produced in the reaction of propylene, ammonia, and oxygen:

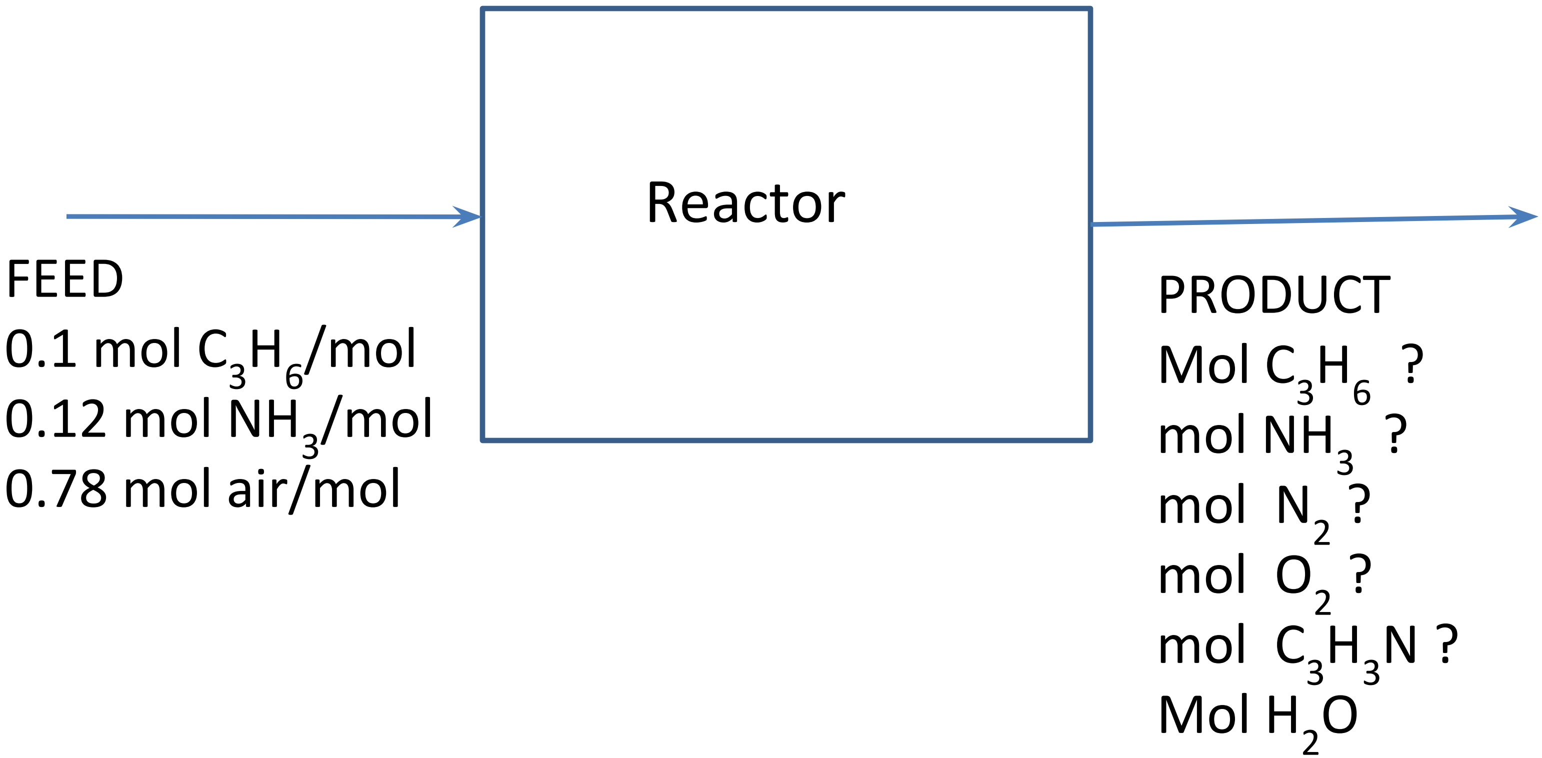
$$C_3H_6 + NH_3 + 3/2\ O_2 \rightarrow C_3H_3N + 3H_2O$$

The feed to the reactor contains 10 mol% propylene, 12 mol% ammonia, and 78 mol% air.

A fractional conversion of 30% of the limiting reactant is achieved. Determine the percentages excess of the excess reactants, and the moles of all product components at the outlet of the reactor.

SOLUTION

A simple schematic of the problem using the information given in the statement can be made



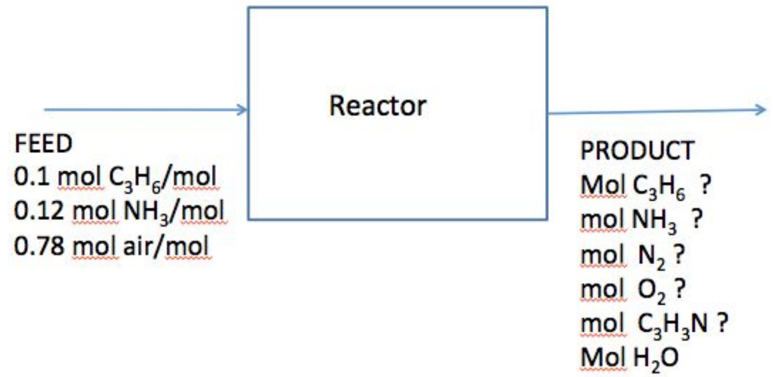
- Step 1

Find which of the reactants is limiting reactant

- Step 2

Based on the moles of limiting reactant converted, calculate the moles of other reactants from stoichiometry.

Basis: 100 mol of feed



N_2 in air = 78 * 0.79 = 61.6 mol

O_2 in air =78*0.21 = 16.4 mol

Reaction: $C_3H_6 + NH_3 + 3/2\ O_2 \rightarrow C_3H_3N + 3H_2O$

For 10 mol of C_3H_6 , NH_3 required is 10 mol

For 10 mol of C_3H_6 , O_2 required is 15 mol

Therefore

% excess of NH_3 = {(NH_3 fed-NH_3 required)/NH3 required}*100

= ((12-10)/10}*100 = 20%

% excess of O_2 ={(O_2 fed-O_2 required)/O_2 required}*100

= {(16.4-15)/15}*100 = 9.3%

- Moles of C_3H_6 in product = 10-3 = 7
- Moles of NH_3 in the product = 12-3=9
- Moles of C_3H_3N in the product = 3
- Moles of H_2O in the product = 9
- Moles of O_2 in the product = 16.4-4.5= 11.9
- Moles of N_2 in the product = 61.6

Yield

It is defined as the moles of product formed to the moles that would have been formed if there were no side reactions and the reaction were complete.

Selectivity

It is the ratio of moles of desired product formed to the moles of undesired product formed.

Exercise

The reactions

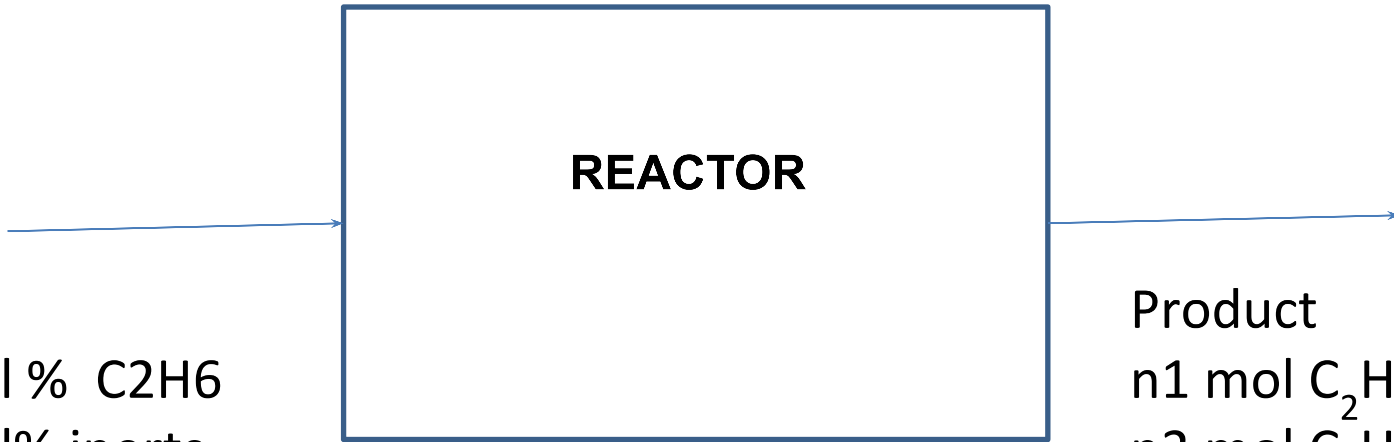
$$C_2H_6 \longrightarrow C_2H_4 + H_2$$

$$C_2H_6 + H_2 \longrightarrow 2CH_4$$

take place in a continuous reactor at steady state. The feed contains 85 mol% ethane and balance inerts. The fractional conversion of ethane is 0.501, and the fractional yield of ethylene is 0.471. Calculate the molar compositions of the product gas and the selectivity of ethylene to methane production.

Solution

Basis: 100 Mol of feed



FEED
85 mol % C2H6
15 mol% inerts

Product
n1 mol C_2H_6
n2 mol C_2H_4
n3 mol H_2
n4 mol CH_4
n5 mol inerts

ethane (C_2H_6) converted = 85*0.501 = 42.6 mol

(C_2H_6) in product = n1 = 85-42.6 = 42.4 mol

Maximum possible ethylene (C_2H_4) that could have formed = 85 mol (from definition of yield)

Yield = ethylene formed/ maximum ethylene that could have been formed

Therefore,

Ethylene formed = yield* maximum possible

= 0.471*85 = 40 mol = n2

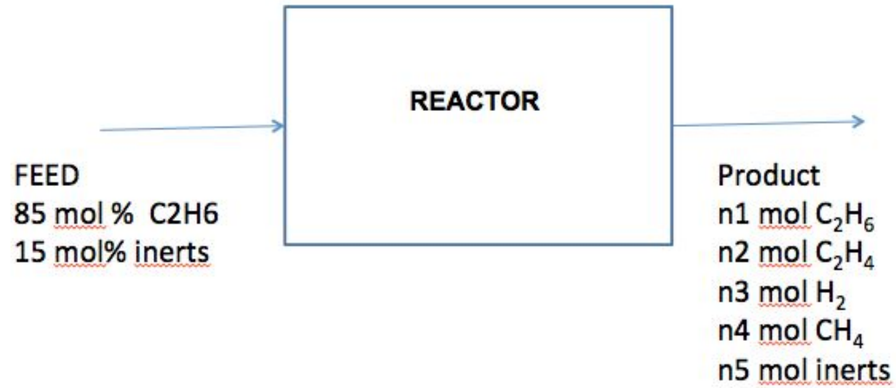
- Therefore, 40 mol of ethane are consumed in reaction 1 (as 1 mol of ethane gives 1 mol of ethylene)

And

Ethane consumed in reaction 2 is

= total moles of ethane converted – moles of ethane converted in reaction 1

=42.6-40 = 2.6 mol



$$C_2H_6 \rightarrow C_2H_4 + H_2$$
$$C_2H_6 + H_2 \rightarrow 2CH_4$$

Therefore,

n2 = 40 mol

n3 = 40-2.6 =37.4 mol

n4 = 2*2.6 = 5.2 mol

n5 = 15 mol

Total moles of product stream

$= n1+n2+n3+n4+n5 = 42.4+40+37.5+5.2+15$

$= 140.1$ mol

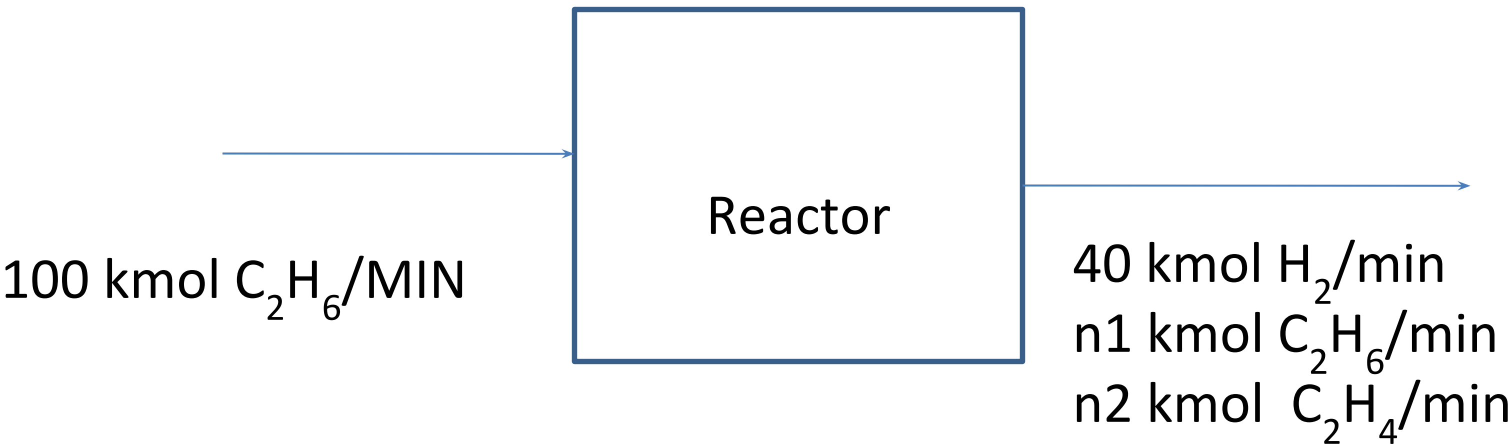
Composition of the product stream:

- C_2H_6 = (42.4/140.1)*100= 30.3%
- C_2H_4 = (40/140.1)*100 = 28.6%
- H_2 = (37.5/140.1)*100= 26.7%
- CH_4 = (5.2/140.1)*100 =3.7%
- Inerts = (15/140.1)*100= 10.7%

Problem (molecular and elemental balances)

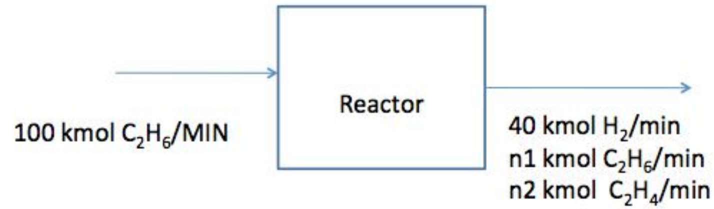
- Consider the following process:

$$C_2H_6 \longrightarrow C_2H_4 + H_2$$



- Solve for n1 and n2 using molecular species and elemental species balances.

We may write the following molecular species balances:



H_2 balance:

Generation of H_2 = output of H_2 = 40 kmol/min

C_2H_6 Balance:

Input = output +consumption

100 = n1+40 ; n1 = 60 kmol/min

C_2H_4 balance:

Generation of C_2H_4 = output of C_2H_4

40 = n2

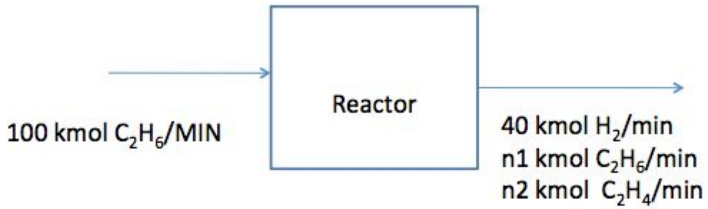
- Or we may write elemental species balance

There are two species: C & H

C balance:

Mol C In = mol C out

So, 200 = 2n1+2n2 (Since 100 Kmol of C_2H_6 have 200 Kmol of C)



H balance:

Mol H In = mol H out

600 = 40*2+ n1*6+n2*4

Solving the above two equations simultaneously

n1 = 60 kmol/min

n2 = 40 kmol/min