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

Course: Material and Energy Balances UCH301

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Solving Atomic Species Balances

- Sometimes in a problem statement the data is given in such a manner that atomic species balances are needed for the solution

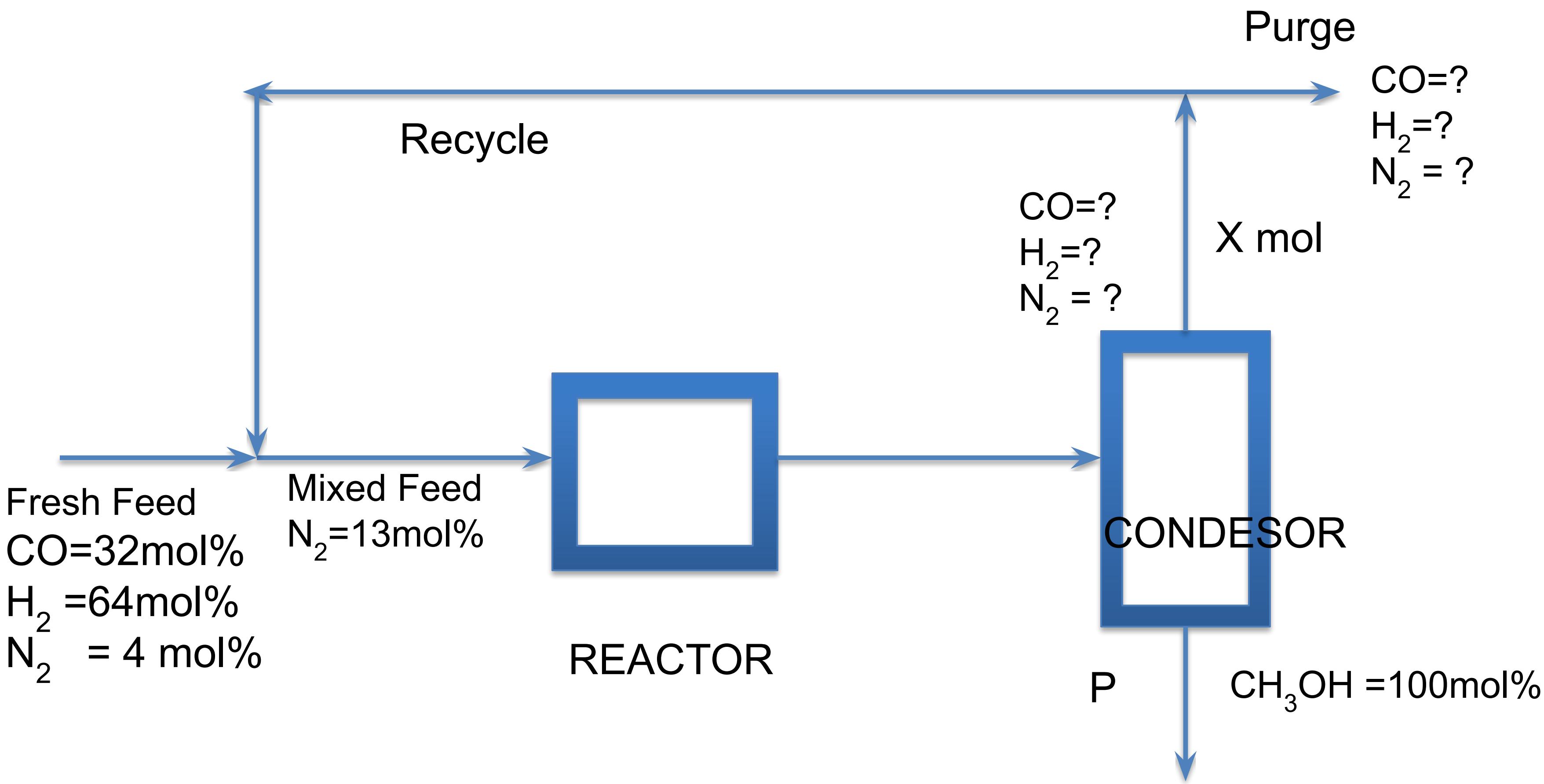
PROBLEM

- Methanol (CH_3OH) is synthesized from CO and H_2 in a catalytic reactor. The fresh feed to the process contains 32% CO, 64% H_2, and 4% N_2. This stream is mixed with a recycle stream in a ratio 5 mol recycle/ 1 mol fresh feed to produce the feed to the reactor, which contains 13% N_2. A low single-pass conversion is achieved in the reactor. The reactor effluent goes to a condenser from which two streams emerge: a liquid product stream containing the entire methanol formed in the reactor, and a gas stream containing all CO, H_2 and N_2 leaving the reactor.

The gas stream is split into two fractions: one is removed from the process as a purge stream, and the other is the recycle stream that combines with the fresh feed. Calculate the production rate of methanol (mol/h), the molar flow rate and compositions of the purge stream, and the overall and single-pass conversions.

Reaction: $CO + H_2 \rightarrow CH_3OH$

SOLUTION



Purge
CO=?
H_2=?
N_2 = ?
Recycle
CO=?
H_2=?
N_2 = ?
X mol
Fresh Feed
CO=32mol%
H_2 =64mol%
N_2 = 4 mol%
Mixed Feed
N_2=13mol%
REACTOR
CONDESOR
P
CH_3OH =100mol%

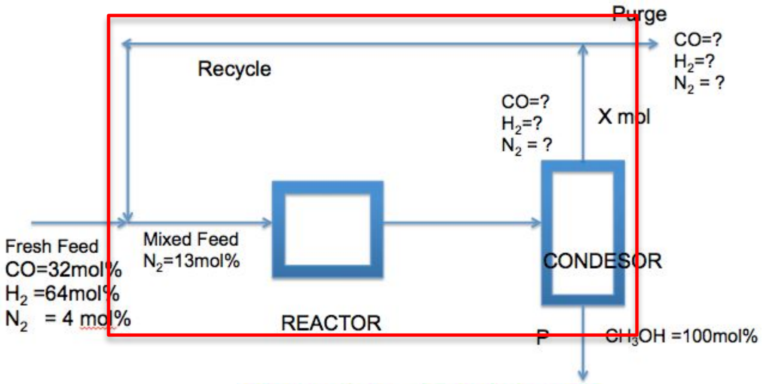
Solution

- Basis: 100 kmol of fresh feed

Data is given such that atomic species balance is necessary

Let P moles of product methanol are produced

Atomic species balances:



$CO + H_2 \rightarrow CH_3OH$

C balance:

$$32 = Purge*x_{co,Purge} + P*X_{CH3OH,P}$$

H balance:

$$64*2 = 4P + 2*Purge*(1 - x_{co,Purge} - x_{N2,Purge})$$

N_2 balance:

$$4 = Purge*x_{N2,Purge}$$

N_2 Balance on mixing point:

N_2 in feed $+N_2$ in R = N_2 in MF

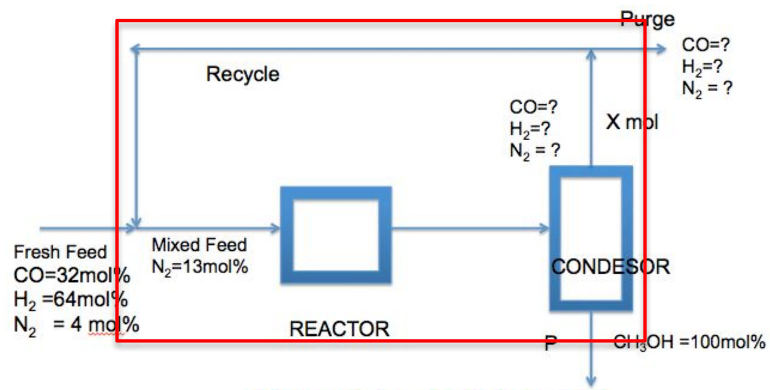
$4 + 500 * x_{N2,R} = 0.13 * MF$

MF= FF+ R =100+500= 600

$x_{N2,R} = ((0.13*600)-4)/500 =$ **0.148**

From N_2 balance ($4 = Purge * x_{N2,purge}$):

Purge = 27 kmol



$CO + H_2 \rightarrow CH_3OH$

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Solving C and H balance simultaneously

$$32 = 27 * X_{CO,Purge} + P$$ C balance

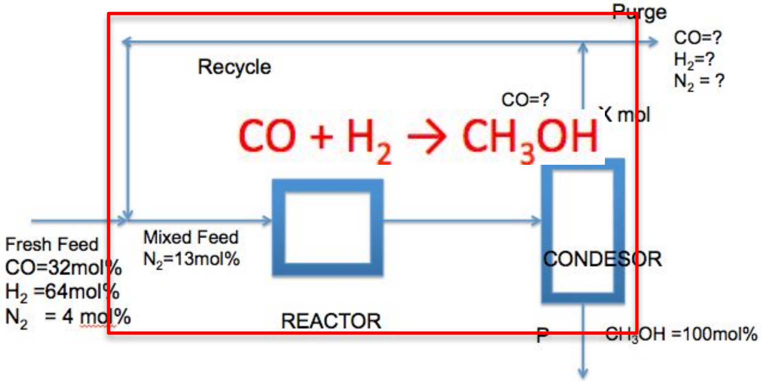
$$2*64 = 27*2*(1-0.148-x_{CO,purge}) + 4*P$$ H balance

Solving for $X_{CO,P}$ & P

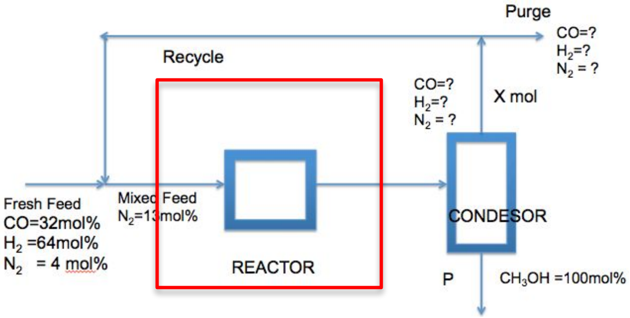
P = 24.33 kmol

$x_{CO,purge} = \mathbf{0.284}$

$x_{H2,p} = 1 - X_{CO,P} - X_{N2,P} = \mathbf{0.568}$



For calculating Single pass conversion, we need to calculate mol of CO at reactor inlet and Outlet:



CO in Fresh Feed = 100*0.32= 32 kmol

CO in purge = 27*0.284 = 7.668 kmol

CO in Recycle = 500*0.284 = 142 kmol

CO in X = 142+7.668 = 149.668 mol

$CO + H_2 \rightarrow CH_3OH$

CO in Gross product = CO in X

CO in X = (500+27)*0.284=149.67 mol

Single pass conversion = 100* (CO in MF-CO in GP)/CO in MF

100*{(142+32)-149.668}/ {142+32}

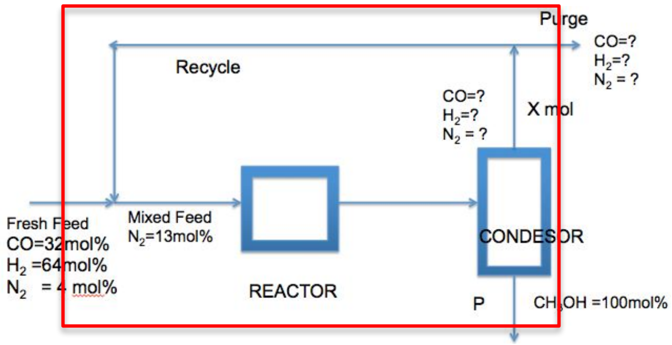
= **13.98%**

Total mol of G.P. = R+Purge+P = 500+27+24.33 = 551.33 mol

Overall conversion=100* (CO in FF-CO in (P+Purge)}/CO in FF

CO in Purge = Purge*$X_{CO,Purge}$ = 27*0.284 =7.668

={(32 –(0+7.668)}/32 = **76%**



$CO + H_2 \rightarrow CH_3OH$

Try Yourself

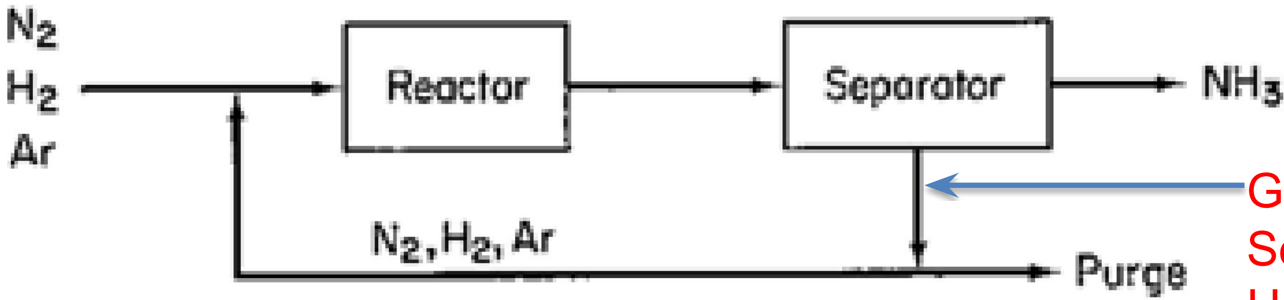
A fresh feed composed of 75.16% H_2, 24.57% N_2 and 0.27% Ar is mixed with the recycled gas and enters the reactor with a composition of 79.52% H_2. The gas leaving the ammonia separator contains 80.01% H_2 and no ammonia. The product ammonia contains no dissolved gases. Per 100 moles of fresh feed:

(i) How many moles are recycled and purged?

(ii) What is the percent conversion of hydrogen per pass?

Sketch

$$3H_2 + N_2 \longrightarrow 2NH_3$$



Gas from Separator
H_2 =80.01mol%
NH_3 =0 mol%
N_2 = ?
Ar = ?

Fresh Feed=100 mol
N_2 =24.57mol%
H_2 =75.16 mol%
Ar = 0.27mol%

Mixed Feed
H_2 =79.52mol%

HINTS

- As you can see that information about the conversion is not given, you will have to use atomic species balances to solve the problem: N, H, Ar balances for overall process
- Writing N balance is required as N_2 is not an inert component in this process
- As composition of %H_2 in separated gas is given, this value will be same for Recycle and Purge.
- **Do not write total mol balance on the overall process as, mol in = mol out, since moles are not conserved in this process**