CHEMICAL PROCESS CALCULATIONS

(Chemical Reaction Stoichiometry)

Lecture # 16: November 02, 2023

Methane is burned with air in a continuous steady-state combustion reactor to yield a mixture of carbon monoxide, carbon dioxide, and water. The reactions taking place are:

$$CH_4 + 3/2\ O_2 = CO + 2H_2O$$

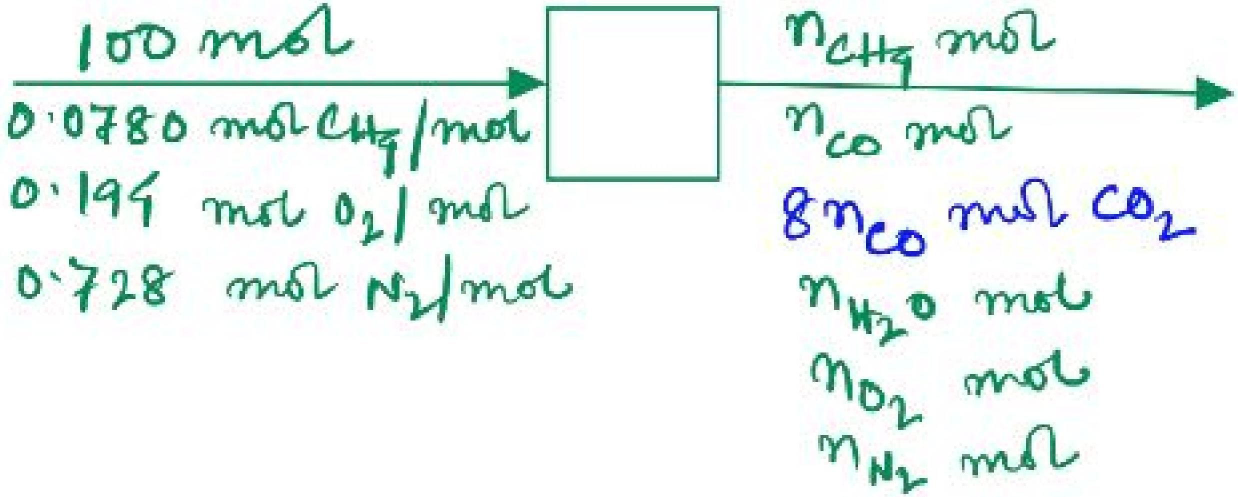
$$CH_4 + 2O_2 = CO_2 + 2H_2O$$

The feed to the reactor contains 7.80 mole% CH_4 , 19.4% O_2 , and 72.8% N_2. The percentage conversion of methane is 90.0%, and the gas leaving the reactor contains 8 mol CO_2 /mol CO.

- Perform degree-of-freedom analysis on the process.
- Calculate the molar composition of the product stream using molecular species balances, atomic species balances, and extents of reaction.

$$CH_4 + 3/2\ O_2 = CO + 2H_2O$$

$$CH_4 + 2O_2 = CO_2 + 2H_2O$$



MSB

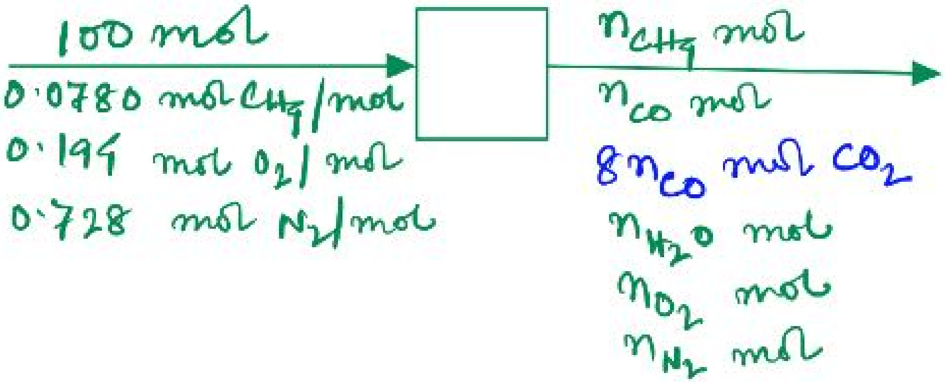
Unknown variables (5)

\+ Independent reactions (2)

− " molecular species (6)

− Additional information (1)
(CH4 conversion)

DOF = 0



ASB

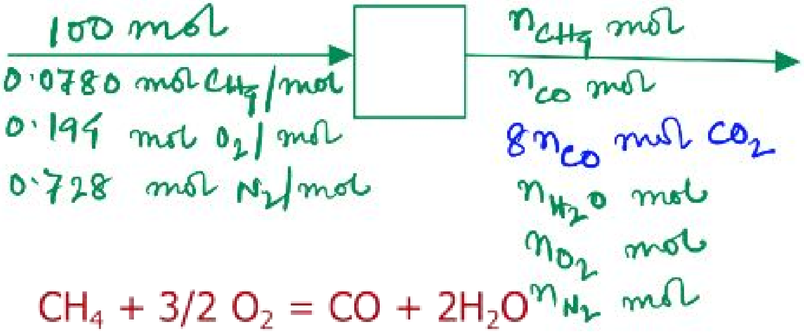
Unknown variables (5)
- Independent atomic species (3)
- Nonreactive molecular species (1)
- Additional information (1)
  (CH_4 conversion)

DOF = 0

EoR

Unknown variables (5)
+ Independent reactions (2)
- EoR expression for species (5)
- Nonreactive molecular species (1)
- Additional information (1)

DOF = 0



$CH_4 + 3/2\ O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$

90% CH_4 conversion

$$n_{CH_4} = (1-0.900)\times 7.8 = 0.78 \text{ mol } CH_4$$

Nonreactive species (N_2) balance

$$\text{input} = \text{output} \Rightarrow n_{N_2} = 72.8 \text{ mol } N_2$$

CO balance:

$$\text{Output} = \text{generation} \Rightarrow n_{CO} = G_{CO,1}$$

CO_2 balance:

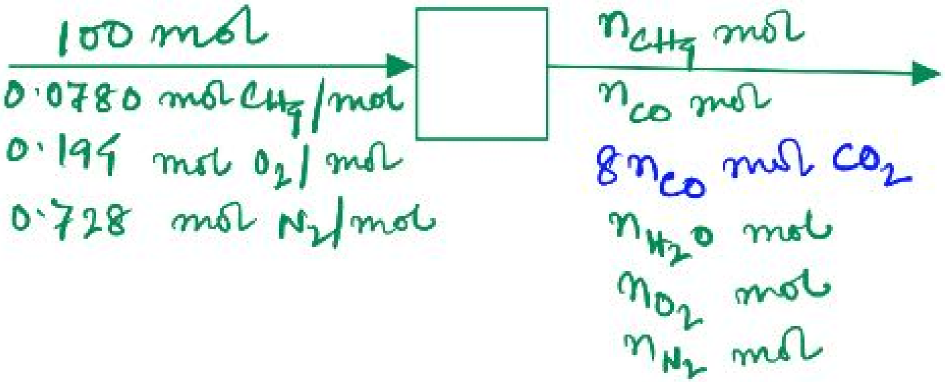
$$\text{output} = \text{generation} \Rightarrow 8n_{CO} = G_{CO_2,2}$$

CH_4 balance:

$$\text{input} = \text{output} + \text{consumption}$$

$$7.8 = 0.780 + G_{CH_4,1} + C_{CH_4,2}$$

$$\Rightarrow 7.02 = G_{CO,1} + G_{CO_2,2}$$



$\Rightarrow \quad 7.02 = n_{CO} + 8n_{CO}$

$\Rightarrow \quad \boxed{n_{CO} = 0.780 \text{ mol } CO}$

$$\Rightarrow \quad \boxed{\begin{aligned} n_{CO_2} &= 8 \times 0.780 \text{ mol } CO_2 \\ &= 6.24 \text{ mol } CO_2 \end{aligned}}$$

H_2O balance:

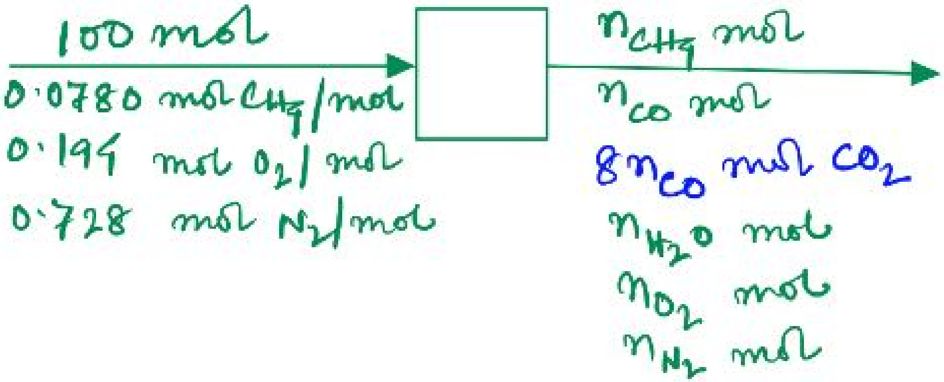
Output = generation

$n_{H_2O} = G_{H_2O,1} + G_{H_2O,2}$

$\Rightarrow \quad n_{H_2O} = G_{CO,1} \times 2 + G_{CO_2,2} \times 2$

$= n_{CO} \times 2 + 8n_{CO} \times 2$

$\Rightarrow \quad \boxed{n_{H_2O} = 14.04 \text{ mol } H_2O}$



$CH_4 + 3/2\ O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$

O_2 balance:

input = output + consumption

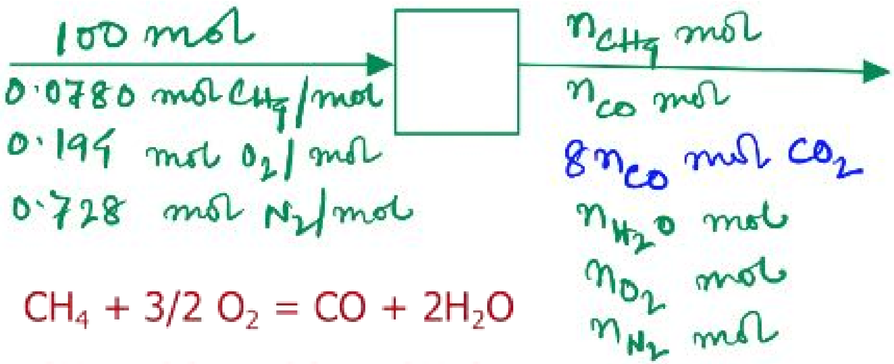
$\Rightarrow 19.4 = n_{O_2} + C_{O_2,1} + C_{O_2,2}$

$\Rightarrow 19.4 = n_{O_2} + G_{CO,1} \times 1.5 + G_{CO_2,2} \times 2$

$\Rightarrow 19.4 = n_{O_2} + n_{CO} \times 1.5 + 8n_{CO} \times 2$

$\Rightarrow \boxed{n_{O_2} = 5.75 \text{ mol } O_2}$

Atomic Species Balances



$CH_4 + 3/2\, O_2 = CO + 2H_2O$

$CH_4 + 2O_2 = CO_2 + 2H_2O$

C balance

input = output

$$7.8 = \underbrace{0.78}_{CH_4} + \underbrace{n_{CO}}_{CO} + \underbrace{8n_{CO}}_{CO_2}$$

$\Rightarrow$ $n_{CO} = 0.78$ mol CO

$n_{CO_2} = 8 \times 0.78 = 6.24$ mol CO_2

H balance:

$$7.8 \times 4 = 0.78 \times 4 + n_{H_2O} \times 2$$

$\Rightarrow$ $n_{H_2O} = 14.04$ mol H_2O

O balance:

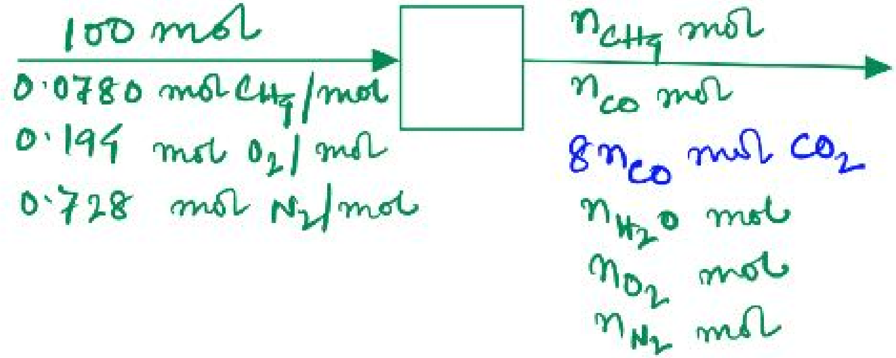
$$19.4 \times 2 = n_{O_2} \times 2 + 0.78 \times 1 + 6.24 \times 2 + 14.04 \times 1$$

$\Rightarrow$ $n_{O_2} = 5.75$ mol O_2

Extents of Reaction

$$n_{CH_4} = 0.78 = 7.8 - \xi_1 - \xi_2$$

$$\Rightarrow \xi_1 + \xi_2 = 7.02$$



$$n_{CO} = \xi_1$$

$$n_{CO_2} = \xi_2 = 8n_{CO} = 8\xi_1$$

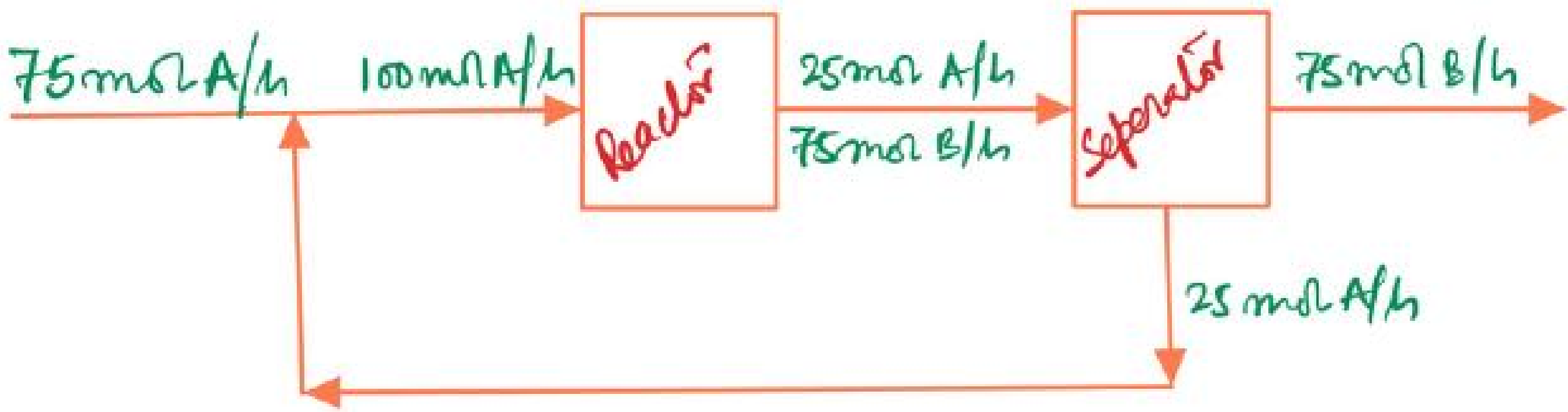
$$n_{H_2O} = 2\xi_1 + 2\xi_2$$

$$n_{O_2} = 19.4 - 1.5\xi_1 - 2\xi_2$$

$$\xi_1 = 0.78$$

$$\xi_2 = 6.24$$

Recycle and conversion



$$\text{Overall conversion} = \frac{\text{reactant input} - \text{reactant output}}{\text{reactant input}}$$ || Process

$$\text{Single pass conversion} = \frac{\text{reactant input} - \text{reactant output}}{\text{reactant input}}$$ || Reactor

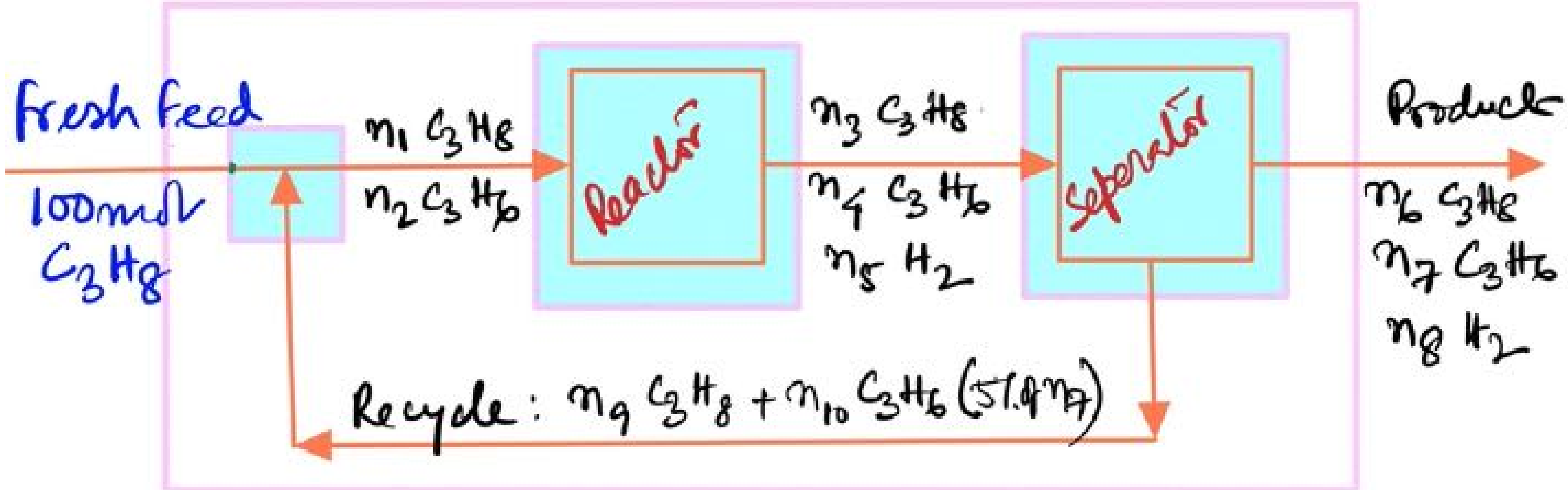
$$C_3H_8 \rightarrow C_3H_6 + H_2$$

Overall conversion of propane : 95%

Seperation after reaction

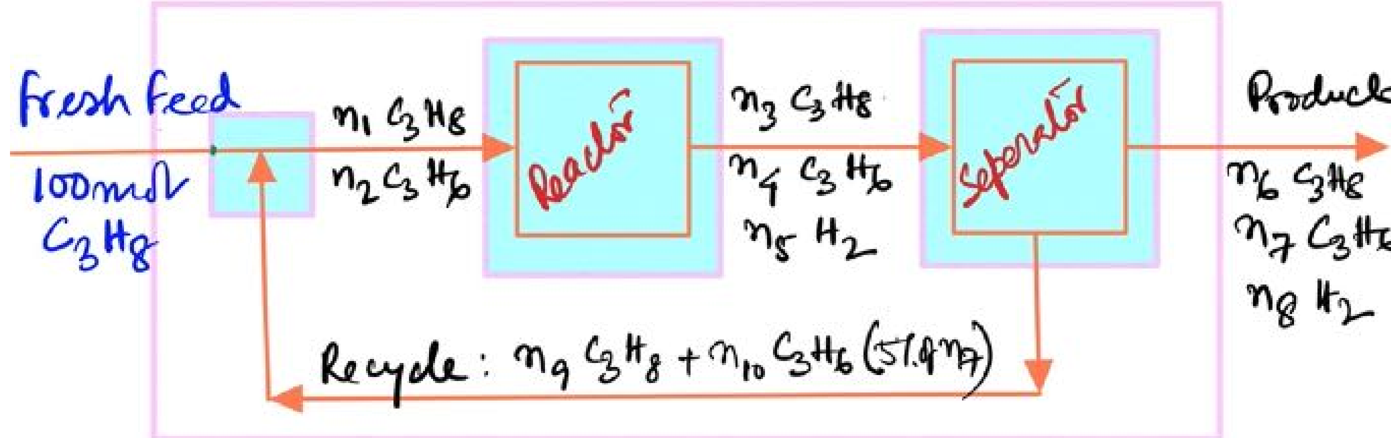
→ H_2, C_3H_6 & 0.555% of C_3H_8 leaving the reactor [Product]

→ unreacted C_3H_8 & 5% of C_3H_6 in the product stream [Recycle]



Overall System

$$DOF = 3\,(n_6, n_7, n_8) - 2\,(C, H) - 1\,(\text{conversion})$$
$$= 0$$



Mixing Point

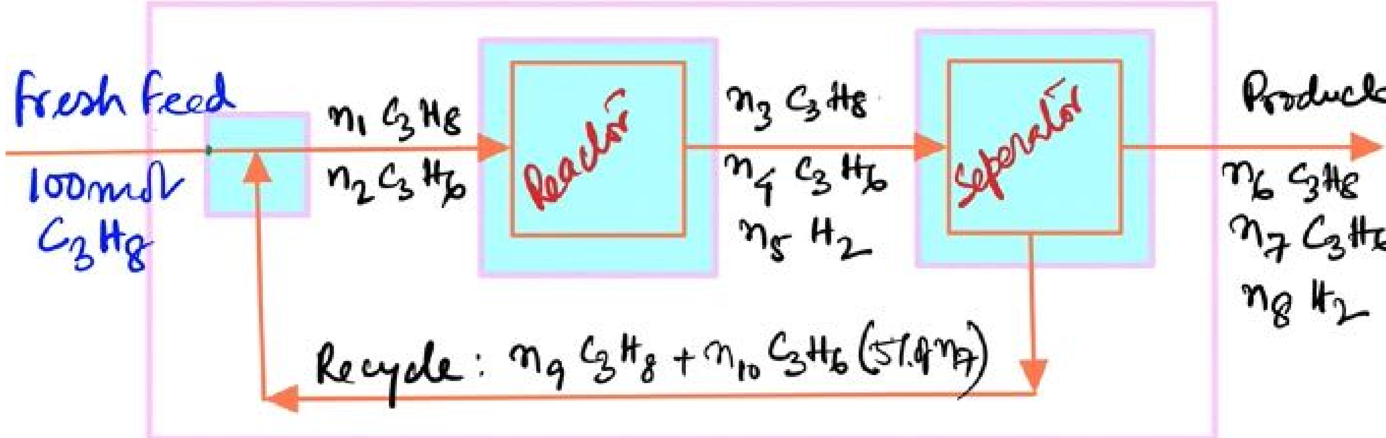
$$DOF = 4(n_9, n_{10}, n_1, n_2) - 2(C_3H_8, C_3H_6) = 2$$

Reactor

$$DOF = 5(n_1, n_2, n_3, n_4, n_5) - 2(C, H) = 3$$

Separator

$$DOF = 5(n_3, n_4, n_5, n_9, n_{10}) - 3(C_3H_8, C_3H_6, H_2)$$
$$- 2(n_6 = 0.00555 n_3 \ \& \ n_{10} = 0.05 n_7)$$
$$= 0$$



95% Overall conversion of Propane

$\Rightarrow$ 5% unconverted

$\Rightarrow$ $n_6 = 0.05 \times 100 = \underline{\underline{5 \text{ mol}}}\ C_3H_8$

Overall C balance

$100 \times 3 = n_6 \times 3 + n_7 \times 3 \Rightarrow n_7 = \underline{\underline{95}}\text{ mol } C_3H_6$

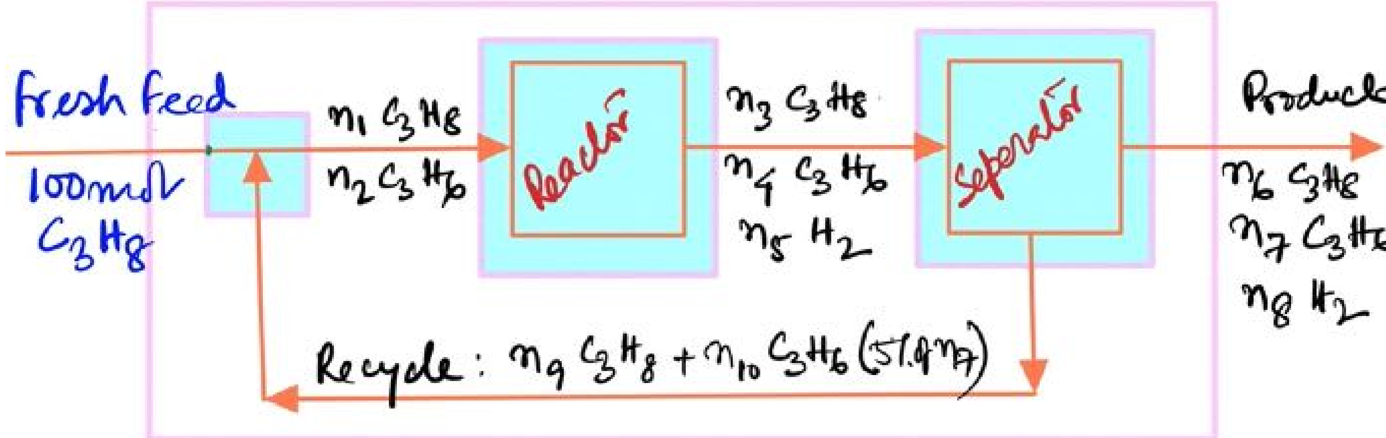
Overall H balance

$100 \times 8 = n_6 \times 8 + n_7 \times 6 + n_8 \times 2$

$\Rightarrow$ $n_8 = \underline{\underline{95}}\text{ mol } H_2$

Product composition

$\left.\begin{array}{l} 5 \text{ mol } C_3H_8 \\ 95 \text{ mol } C_3H_6 \\ 95 \text{ mol } H_2 \end{array}\right\}$ $\begin{array}{l} 2.6\%\ C_3H_8 \\ 48.7\%\ C_3H_6 \\ 48.7\%\ H_2 \end{array}$



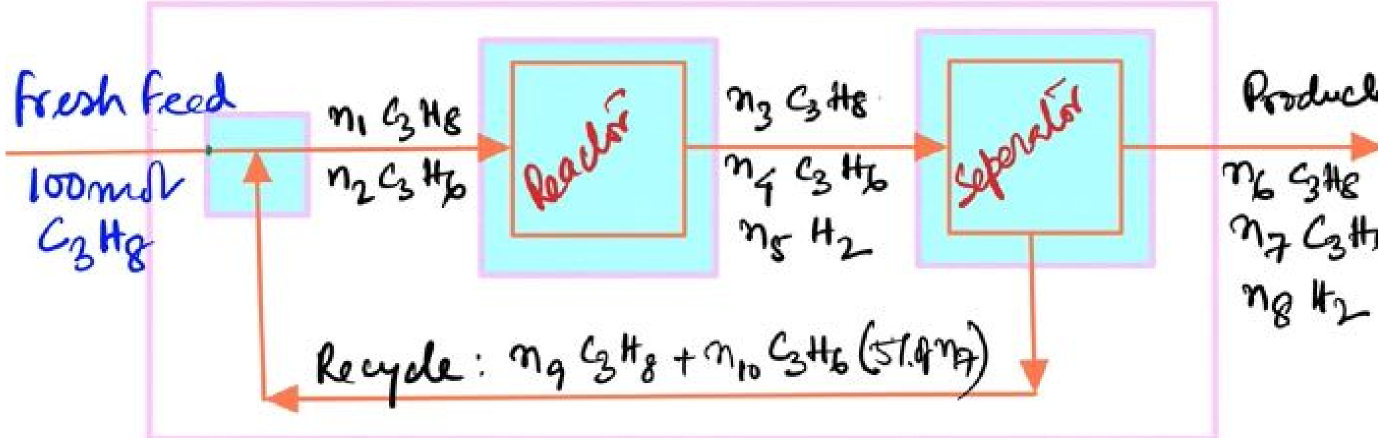
$n_6 = 0.00555\, n_3 \Rightarrow n_3 = 900.9$ mol C_3H_8

$n_{10} = 0.05\, n_7 \Rightarrow n_{10} = 4.75$ mol C_3H_6

Propane balance on Separator

$n_3 = n_6 + n_9 \Rightarrow n_9 = 895$ mol C_3H_8

Similarly n_4 & n_5



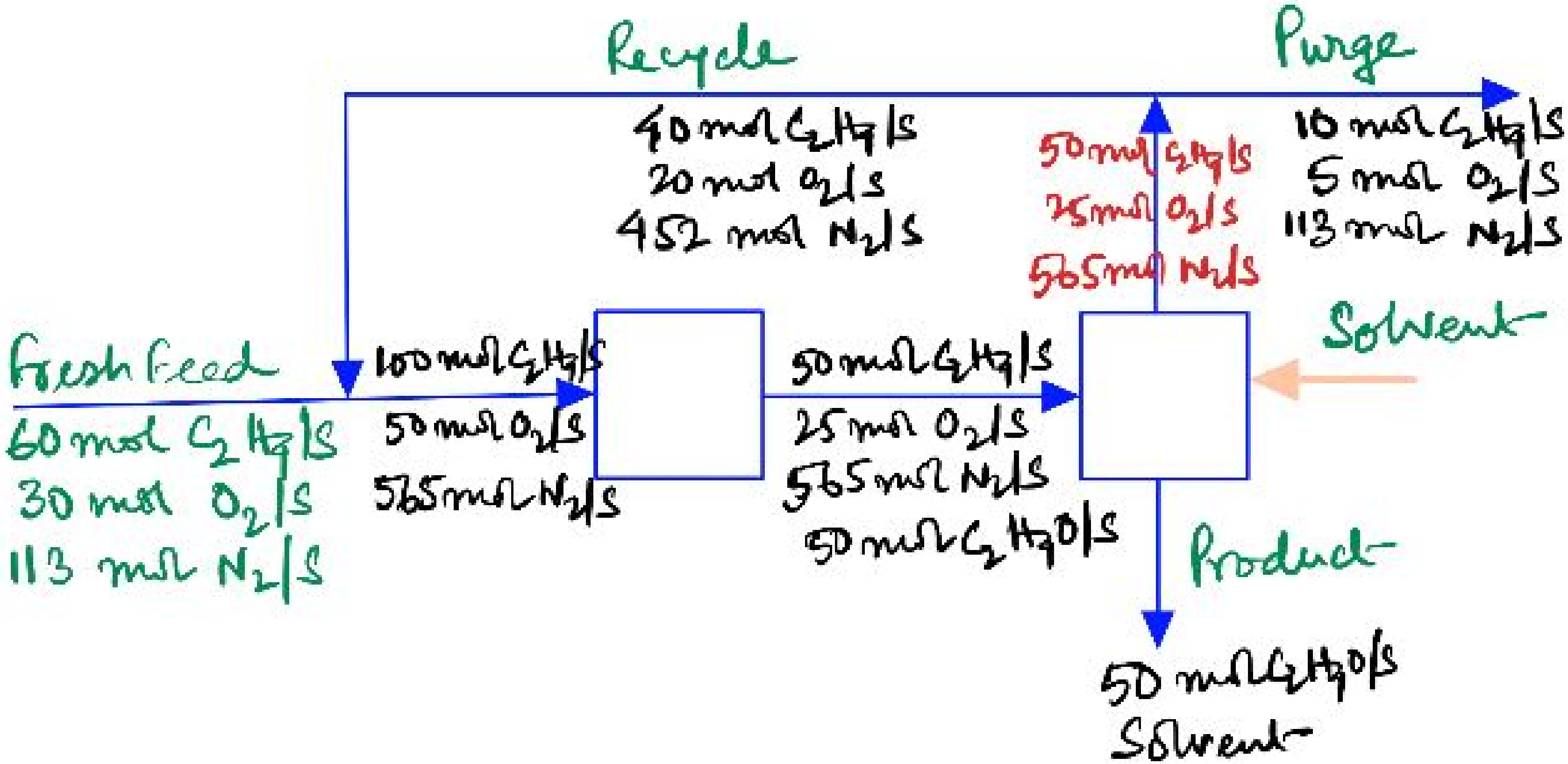
Propane balance on mixing point

$$100 + n_9 = n_1 \Rightarrow n_1 = 995 \text{ mol } C_3H_8$$

$$\text{Recycle ratio} = \frac{n_9 + n_{10}}{100} = 9.00 \frac{\text{mol recycle}}{\text{mol fresh feed}}$$

$$\text{Single pass conversion} = \frac{n_1 - n_3}{n_1} \times 100\% = 9.6\%$$

Purging system



Methanol is synthesized from carbon monoxide and hydrogen in a catalytic reactor. The fresh feed to the process contains 32.0 mole% CO, 64.0% H_2, and 4.0% 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 13.0 mole% N_2. A low single-pass conversion is attained in the reactor. The reactor effluent goes to a condenser from which two streams emerge: a liquid product stream containing essentially all the methanol formed in the reactor, and a gas stream containing all the 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 to the reactor.

For a basis of 100 mol fresh feed/h, calculate the production rate of methanol (mol/h), the molar flow rate and composition of the purge gas, and the overall and single-pass conversions.