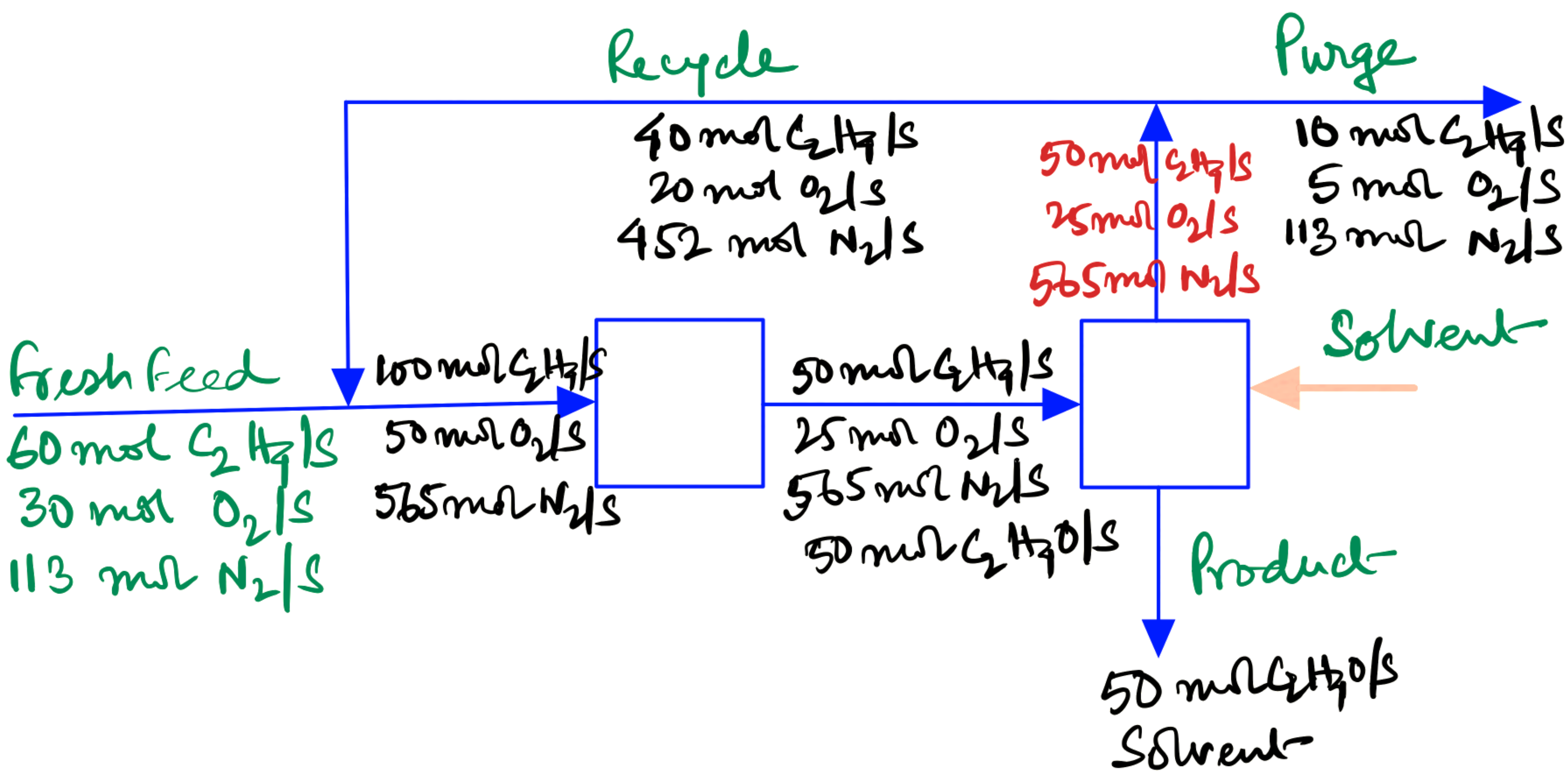
CHEMICAL PROCESS CALCULATIONS

(Reactive process balance)

Lecture # 16: October 27, 2022

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.

Combustion Reactions

- Complete combustion
- Incomplete / Partial combustion
- Composition on a **wet** basis
- Composition on a **dry** basis
- Stack or flue gas
- Orsat analysis
  - a technique for stack-gas analysis - dry-basis composition
- Theoretical and excess oxygen and air

Combustion Reactions

$$C + O_2 \rightarrow CO_2$$

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

$$C_3H_8 + \frac{7}{2}O_2 \rightarrow 3CO + 4H_2O$$

$$CS_2 + 3O_2 \rightarrow CO_2 + 2SO_2$$

$$N_2 \rightarrow 78 \cdot 03\%$$
$$O_2 \rightarrow 20 \cdot 99\%$$
$$Ar \rightarrow 0 \cdot 94\%$$
$$CO_2 \rightarrow 0.03\%$$
$$H_2, He, Ne, Kr, Xe \rightarrow 0 \cdot 01\%$$

Average molecular weight = 29.0

$$N_2 \rightarrow 79\%$$
$$O_2 \rightarrow 21\%$$

$$\frac{3 \cdot 76 mol N_2}{1 mol O_2}$$

Combustion Reactions

$N_2 \rightarrow 60.0\%$
$CO_2 \rightarrow 15.0\%$
$O_2 \rightarrow 10.0\%$
Rest H_2O

$\Rightarrow$ Molar composition on dry basis ?

Dry gas = 85.0 mol

$N_2 \rightarrow \frac{60.0}{85.0} = 0.706$ mol N_2/mol dry gas

$CO_2 \rightarrow \frac{15.0}{85.0} = 0.176$ mol CO_2/mol dry gas

$O_2 \rightarrow \frac{10.0}{85.0} = 0.118$ mol O_2/mol dry gas

Combustion Reactions

$N_2 \rightarrow 65\%$
$CO_2 \rightarrow 14\%$
$CO \rightarrow 11\%$
$O_2 \rightarrow 10\%$

$\Rightarrow$ Wet basis composition?

$\boxed{107.53 \text{ mol wet gas}}$

mole fraction of $H_2O = 0.0700$

$$y_{H_2O} = \frac{7.53}{107.53} \text{ mol } H_2O / \text{mol wet gas}$$

$$\frac{0.0700 \text{ mol } H_2O}{\text{mol wet gas}} \Rightarrow \frac{0.930 \text{ mol dry gas}}{\text{mol wet gas}}$$

$$\Rightarrow \frac{0.0700 \text{ mol } H_2O}{0.930 \text{ mol dry gas}} = \frac{0.0753 \text{ mol } H_2O}{\text{mol dry gas}}$$

$$\% \text{ excess air} = \frac{\text{moles air fed} - \text{mole air theoretical}}{\text{moles air theoretical}}$$

Combustion Reactions

100 mol/h C_4H_{10}
+
5000 mol/h air

$\Rightarrow$ % excess air ?

$$\% \text{ excess air} = \frac{5000 - 3094}{3094} \times 100\% = 61.6\%$$

$$C_4H_{10} + \frac{13}{2} O_2 \rightarrow 4CO_2 + 5H_2O$$

$$(\dot{n}_{O_2})_{Theo} = \frac{100 \text{ mol } C_4H_{10}}{h} \times \frac{6.5 \text{ mol } O_2}{\text{mol } C_4H_{10}}$$

$$= 650 \text{ mol } O_2/h$$

$$(\dot{n}_{air})_{Theo} = \frac{650 \text{ mol } O_2}{h} \times \frac{4.76 \text{ mol air}}{\text{mol } O_2}$$

$$= 3094 \frac{\text{mol air}}{h}$$

Balance on combustion reactions

- Requirement of theoretical oxygen does not depend on the amount of fuel actually burned
- % excess air calculation does not depend on either the amount of oxygen consumed or the reaction nature (partial or complete combustion)
- unreacted fuel and oxygen
- water, carbon dioxide, carbon monoxide
- nitrogen (combusted with air and not with pure oxygen)

$\boxed{C_2H_6 + 50\% \text{ excess air}}$

% conversion of $C_2H_6 = 90\%$

25% $C_2H_6 \rightarrow CO$

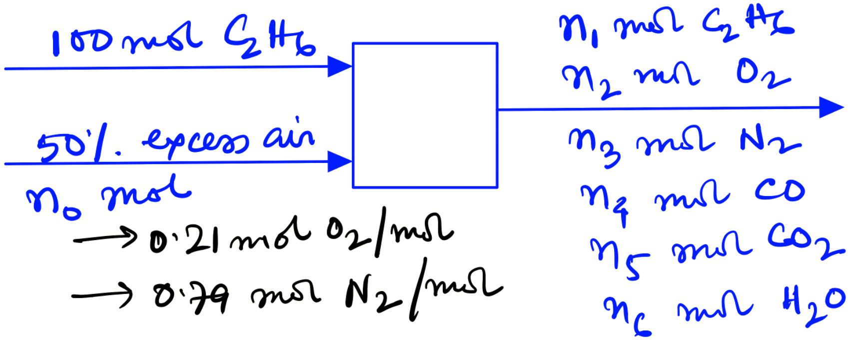
75% $C_2H_6 \rightarrow CO_2$

Molar composition of stack gas on a dry basis & mole ratio of water to dry gas?

$$C_2H_6 + \frac{7}{2}O_2 \longrightarrow 2CO_2 + 3H_2O$$

$$C_2H_6 + \frac{5}{2}O_2 \longrightarrow 2CO + 3H_2O$$

Basis of calculation: 100 mol C_2H_6 feed



DOF analysis

No. of unknowns : 7 $(n_0, n_1, \cdots n_6)$

− No. of atomic balance : 3 (C, H, O)

− N_2 balance : 1

− Excess air information : 1

− C_2H_6 conversion : 1

− CO/CO_2 specification : 1

DOF = 0

$$(n_{O_2})_{Theo} = 100 \times 3.5 = 350 \text{ mol } O_2$$

$$(n_{O_2})_{feed} = 1.5 \times 350 = 0.21\, n_0$$

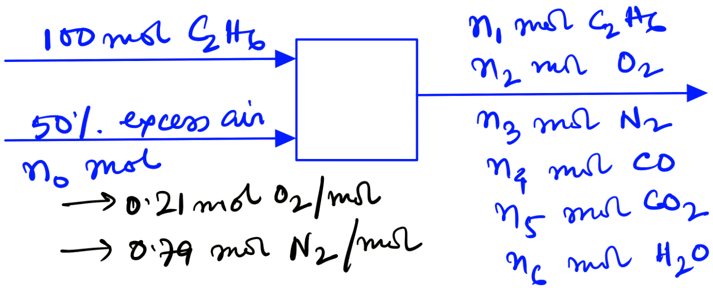
$$\Rightarrow n_0 = 2500 \text{ mol air}$$

10% unreacted C_2H_6

$$n_1 = 0.100 \times 100 = 10.0 \text{ mol } C_2H_6$$

90.0 mol C_2H_6 reacted.

Basis of calculation: 100 mol C_2H_6 feed



$$(0.25 \times 90) \times 2 = n_4$$ [from stoichiometry]

$\Rightarrow n_4 = 45.0$ mol CO

$\Rightarrow n_5 = 135.0$ mol CO_2

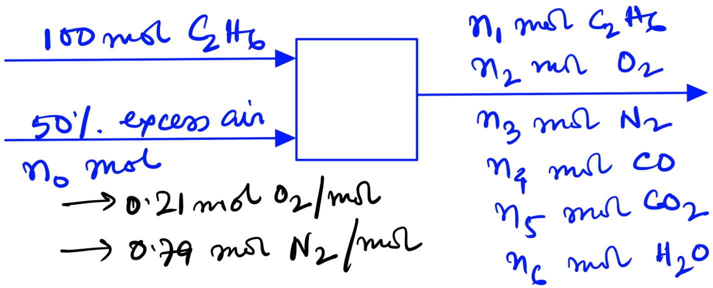
$n_3 = 0.79 \times 2500 = 1975$ mol N_2

Atomic H balance

$$100 \times 6 = 10 \times 6 + n_6 \times 2$$

$\Rightarrow n_6 = 270$ mol H_2O

Basis of calculation: 100 mol C_2H_6 feed



Atomic O balance

$$2 \times 0.21 n_0 = 2 \times 525 = n_2 \times 2 + 45 \times 1 + 135 \times 2 + 270 \times 1$$

$$\Rightarrow n_2 = 232 \text{ mol } O_2$$

$n_1 = 10$ mol C_2H_6
$n_2 = 232$ mol O_2
$n_3 = 1975$ mol N_2
$n_4 = 45$ mol CO
$n_5 = 135$ mol CO_2

Dry gas composition

Total dry stack = 2397 mol

$n_6 = 270$ mol H_2O

Total wet gas = 2667 mol