CHEMICAL PROCESS CALCULATIONS

(Material Balance Calculations: Fundamentals & Single Unit)

Lecture # 10: September 15, 2022

Stoichiometry

- Proportion of chemical species that combine with one another
- Relative number of molecules/moles of reactants and products in a reaction
- Number of atoms of any atomic species on both sides of a reaction must be same
- Stoichiometric coefficients
- Stoichiometric ratio

Limiting & Excess Reactant

- Limiting reactant
- Excess reactant
- Fractional excess
- Percentage excess
- Fractional conversion

Limiting & Excess Reactant

$$C_2H_2 + 2H_2 \rightarrow C_2H_6$$

20 kmol acetylene
50 kmol hydrogen
50 kmol ethane

After some time
30 kmol hydrogen
reacted

$$n_{H_2} = (n_{H_2})_0 - 2\xi$$

$$n_{C_2H_2} = (n_{C_2H_2})_0 - \xi$$

$$n_{C_2H_6} = (n_{C_2H_6})_0 + \xi$$

$$\nu_{C_2H_2} = -1$$

$$\nu_{H_2} = -2$$

$$\nu_{C_2H_6} = +1$$

Limiting & Excess Reactant

$$n_{H_2} = (n_{H_2})_0 - 2\xi$$

$$n_{C_2H_2} = (n_{C_2H_2})_0 - \xi$$

$$n_{C_2H_6} = (n_{C_2H_6})_0 + \xi$$

$\nu_{C_2H_2} = -1$

$\nu_{H_2} = -2$

$\nu_{C_2H_6} = +1$

$$\boxed{n_i = n_{i0} + \nu_i \xi}$$

ξ = Extent of reaction

Limiting & Excess Reactant

$$C_3H_6 + NH_3 + \frac{3}{2}O_2 \rightarrow C_3H_3N + 3H_2O$$

Mole composition:

10% propylene, 12% amonia, 78% air

Fractional conversion:

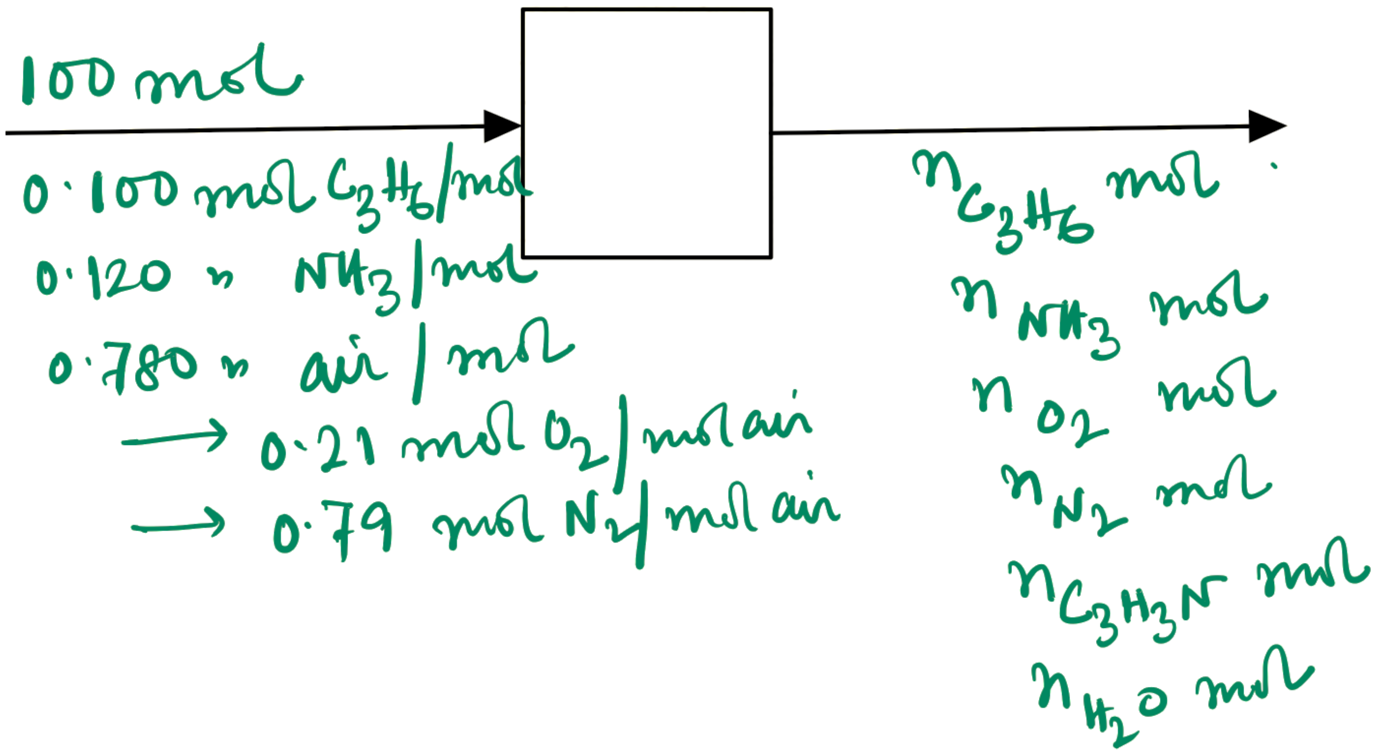
30% of the limiting reactant

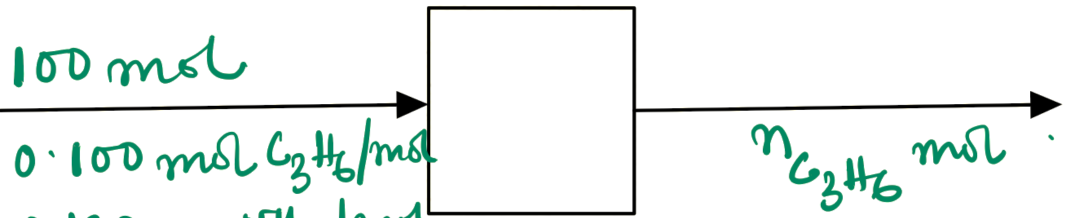
% excess of other reactants

Molar composition of product gas

Limiting & Excess Reactant

$$C_3H_6 + NH_3 + \frac{3}{2}O_2 \rightarrow C_3H_3N + 3H_2O$$





100 mol

0.100 mol C_3H_6/mol

0.120 " NH_3/mol

0.780 " air/mol

$\longrightarrow$ 0.21 mol O_2/mol air

$\longrightarrow$ 0.79 mol N_2/mol air

$n_{C_3H_6}$ mol

n_{NH_3} mol

n_{O_2} mol

n_{N_2} mol

$n_{C_3H_3N}$ mol

n_{H_2O} mol

$$(n_{C_3H_6})_0 = 10.0 \text{ mol}$$

$$(n_{NH_3})_0 = 12.0 \text{ mol}$$

$$(n_{O_2})_0 = 78.0 \times 0.210 = 16.4 \text{ mol}$$

$$(n_{NH_3}/n_{C_3H_6})_0 = \frac{12.0}{10.0} = 1.20$$

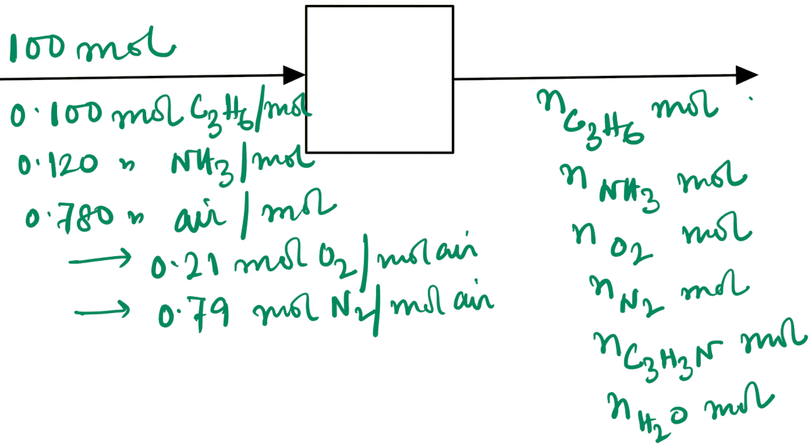
$$(n_{NH_3}/n_{C_3H_6})_{St} = 1/1 = 1$$

$\Rightarrow$ NH_3 is in excess.

$$(n_{O_2}/n_{C_3H_6})_0 = 16.4/10.0 = 1.64$$

$$(n_{O_2}/n_{C_3H_6})_{St} = 1.5/1 = 1.5$$

$\Rightarrow$ O_2 is in excess.



$$\% \text{ excess } NH_3 = \frac{(n_{NH_3})_0 - (n_{NH_3})_{st}}{(n_{NH_3})_{st}} \times 100\%$$

$$= \frac{12.0 - 10.0}{10.0} \times 100\% = 20\%$$

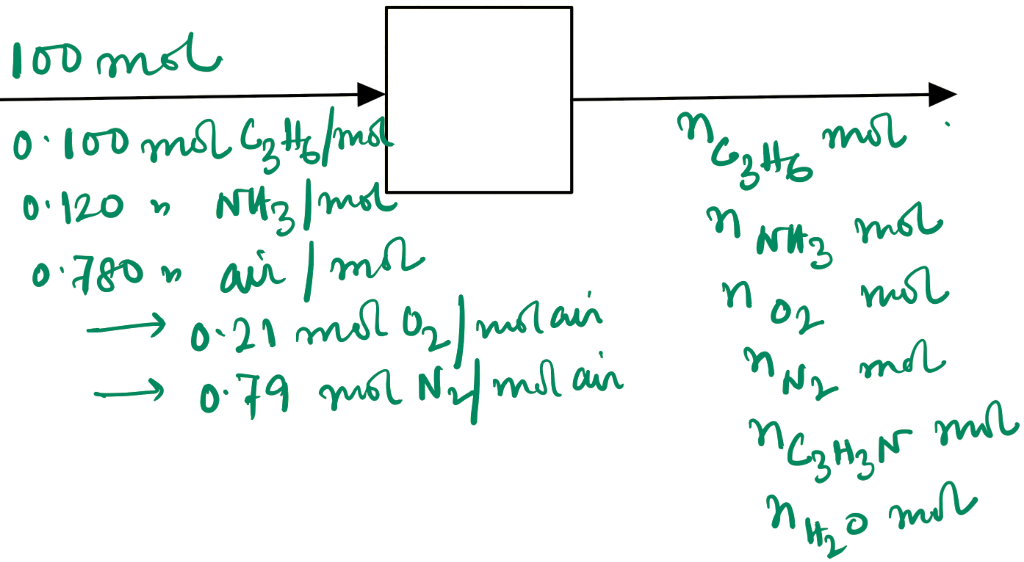
$$\% \text{ excess } O_2 = \frac{16.4 - 15.0}{15.0} \times 100\% = 9.33\%$$

$$(n_{NH_3})_{st} = 10.0 \text{ mol } C_3H_6 \times \frac{1 \text{ mol } NH_3}{1 \text{ mol } C_3H_6}$$

$$= 10.0 \text{ mol } NH_3$$

$$(n_{O_2})_{st} = 10.0 \text{ mol } C_3H_6 \times \frac{1.5 \text{ mol } O_2}{1 \text{ mol } C_3H_6}$$

$$= 15.0 \text{ mol } O_2$$



$$\left(n_{C_3H_6}\right)_{out} = 0.700 \times \left(n_{C_3H_6}\right)_0 = 7.0 \text{ mol}$$

$$\left(n_{C_3H_6}\right)_{out} = 10.0 - \xi$$

$$\Rightarrow \quad \xi = 3.0 \text{ mol}$$

$$n_{NH_3} = 12.0 - \xi \qquad n_{C_3H_3N} = \xi$$

$$n_{O_2} = 16.4 - 1.5\,\xi \qquad n_{H_2O} = 3\,\xi$$

$$n_{N_2} = \left(n_{N_2}\right)_0$$