CHEMICAL PROCESS CALCULATIONS

(Multiple reactions)

Lecture # 12: October 10, 2022

Multiple Reactions, Yield, and Selectivity

- Desired product yield
- Desired product purity
- Yield and Selectivity

$$\text{Yield} = \frac{\text{moles of desired product formed}}{\text{moles that would be formed if there were no side reactions and the limiting reactant were consumed completely}} \times 100\%$$

$$\text{Selectivity} = \frac{\text{moles of desired product formed}}{\text{moles of undesired product formed}}$$

Multiple Reactions, Yield, and Selectivity

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

$$C_2H_6 + H_2 \rightarrow 2CH_4$$

$$C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$$

$$\text{Yield} = \frac{(n_{C_2H_4})_{gen}}{(\nu_{C_2H_4}/\nu_{C_2H_6})(n_{C_2H_6})_{input}} \times 100\%$$

$$\text{Selectivity} = \frac{(n_{C_2H_4})_{gen}}{(n_{CH_4})_{gen}}$$

Yield ⇒ moles of desired product divided by either moles of reactant fed or moles of reactant consumed in the reactor

Multiple Reactions, Yield, and Selectivity

Single reaction : $n_i = n_{i0} + \nu_i \xi$

Multiple reaction: $n_i = n_{i0} + \sum_j \nu_{ij} \xi_j$

$$C_2H_4 + \frac{1}{2}O_2 \longrightarrow C_2H_4O$$

$$C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$$

Multiple Reactions, Yield, and Selectivity

$$(n_{C_2H_4})_{out} = (n_{C_2H_4})_0 - \xi_1 - \xi_2$$

$$(n_{O_2})_{out} = (n_{O_2})_0 - 0.5\xi_1 - 3\xi_2$$

$$(n_{C_2H_4O})_{out} = (n_{C_2H_4O})_0 + \xi_1$$

$$(n_{CO_2})_{out} = (n_{CO_2})_0 + 2\xi_2$$

$$(n_{H_2O})_{out} = (n_{H_2O})_0 + 2\xi_2$$

$$C_2H_4 + \tfrac{1}{2}O_2 \longrightarrow C_2H_4O$$

$$C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$$

Multiple Reactions, Yield, and Selectivity

$$C_2H_6 \rightarrow C_2H_4 + H_2$$

$$C_2H_6 + H_2 \rightarrow 2CH_4$$

Feed: 85.0 mole% ethane and the balance inert

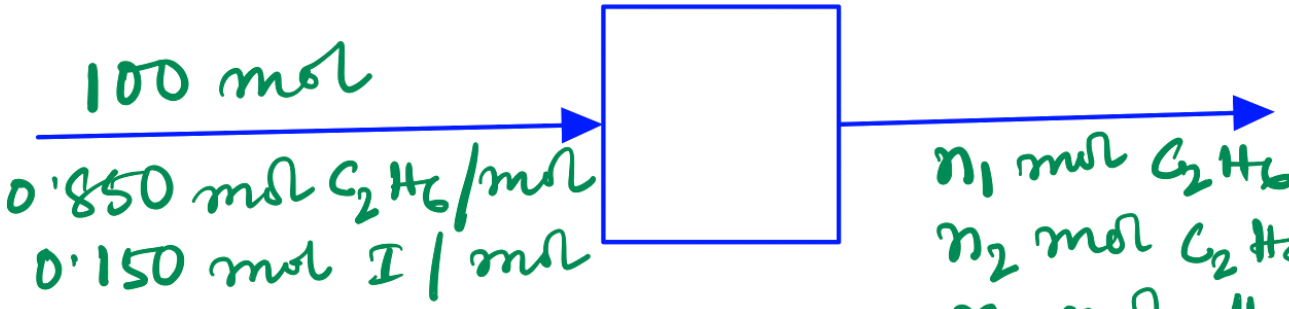
Fractional conversion of ethane = 0.501

Fractional yield of ethylene = 0.471

Calculate

- molar composition of the product gas
- selectivity of ethylene to methane production

Multiple Reactions, Yield, and Selectivity



$$n_1 = 85.0 - \xi_1 - \xi_2$$

$$n_2 = \xi_1$$

$$n_3 = \xi_1 - \xi_2$$

$$n_4 = 2\xi_2$$

$$n_5 = 15.0$$

Multiple Reactions, Yield, and Selectivity

C_2H_6:

Fractional conversion: 0.501

$(1 - 0.501) \times 85.0 = n_1$

$\Rightarrow \boxed{n_1 = 42.4 = 85.0 - \xi_1 - \xi_2}$

C_2H_4:

Fractional yield: 0.471

$0.471 \times 85.0 = n_2$

$\Rightarrow \boxed{n_2 = 40.0 = \xi_1}$ $\Rightarrow \boxed{\xi_2 = 2.6}$

Multiple Reactions, Yield, and Selectivity

$n_3 = \xi_1 - \xi_2 = 37.4$

$n_4 = 2\xi_2 = 5.2$

$n_5 = 15.0$

$n_1 = 42.4$

$n_2 = 40.0$

$n_t = 140.0$

Product

C_2H_6 - 30.3%.

C_2H_4 - 28.6%.

H_2 - 26.7%.

CH_4 - 3.7%.

I - 10.7%.

Selectivity

$= \frac{40.0 \text{ mol } C_2H_4}{5.2 \text{ mol } CH_4} = 7.69 \text{ mol } C_2H_4 / \text{mol } CH_4$