CHEMICAL PROCESS CALCULATIONS

(Material Balance Calculations: Fundamentals & Single Unit)

Lecture # 11: September 19, 2022

Chemical Equilibrium

- Equilibrium composition of the reaction mixture
- Time to reach the onset of equilibrium
- Irreversible reaction
- Reversible reaction

$$C_2H_4 + H_2O \rightleftharpoons C_2H_5OH$$

Chemical Equilibrium

$$CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)$$

$$\frac{y_{CO_2}\, y_{H_2}}{y_{CO}\, y_{H_2O}} = K(T)$$

At $T = 1105\,K$

$K = 1.00$

Feed: { 1 mol CO
2 mol H_2O

Calculate equilibrium composition.

Fractional conversion

Chemical Equilibrium

$$n_{CO} = 1.00 - \xi_e$$

$$n_{H_2O} = 2.00 - \xi_e$$

$$n_{CO_2} = \xi_e$$

$$n_{H_2} = \xi_e$$

$$n_t = 3.00$$

$$y_{CO} = (1.00 - \xi_e)/3.00$$

$$y_{H_2O} = (2.00 - \xi_e)/3.00$$

$$y_{CO_2} = \xi_e/3.00$$

$$y_{H_2} = \xi_e/3.00$$

Chemical Equilibrium

$$\frac{y_{CO_2} y_{H_2}}{y_{CO} y_{H_2O}} = \frac{\xi_e^2}{(1.00 - \xi_e)(2.00 - \xi_e)} = 1.00$$

$$\Rightarrow \quad \xi = 0.667$$

$$y_{CO} = 0.111 \qquad y_{CO_2} = 0.222$$

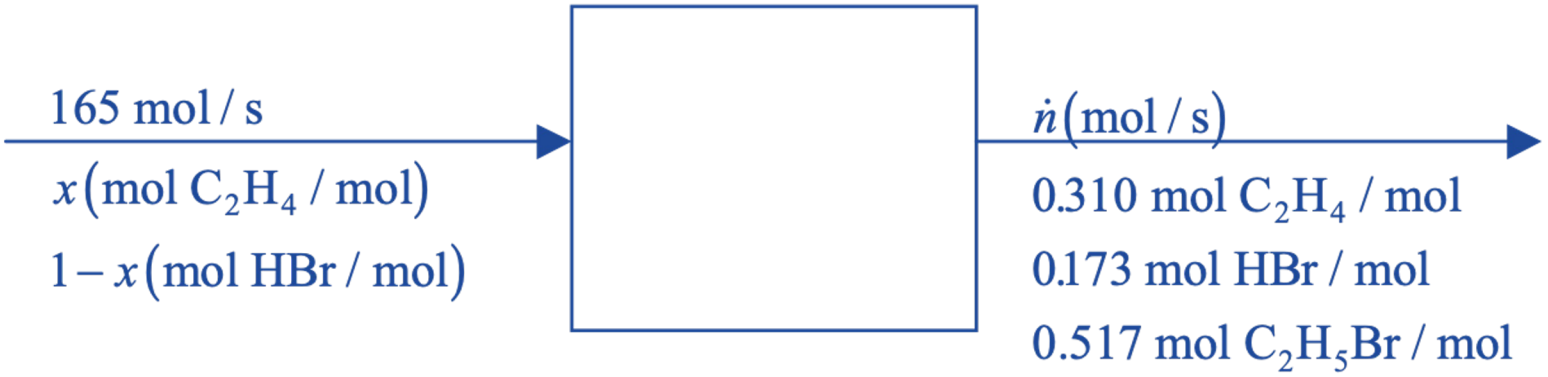
$$y_{H_2O} = 0.444 \qquad y_{H_2} = 0.222$$

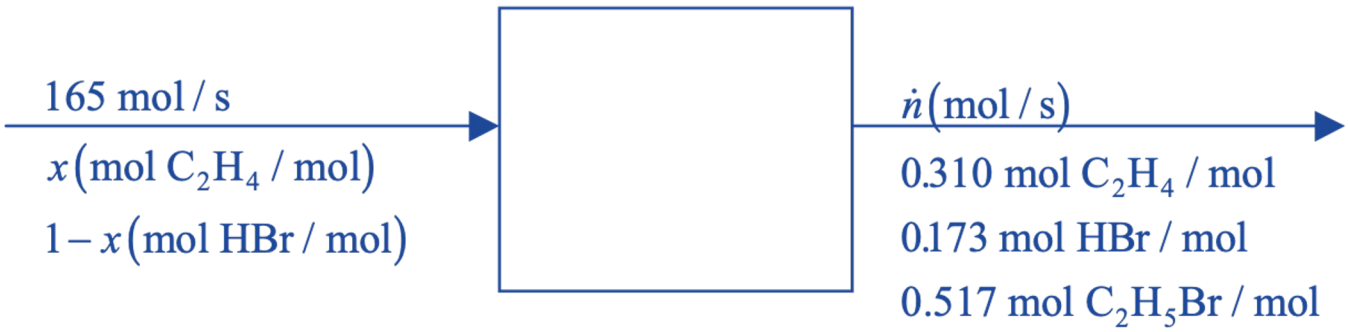
Chemical Equilibrium

$$n_{CO} = (1.00 - 0.667)\ \text{mol} = 0.333\ \text{mol}$$

$$f_{CO} = \frac{(1.00 - 0.333)\ \text{CO reacted}}{1.00\ \text{mol CO fed}} = 0.667$$

The reaction between ethylene and hydrogen bromide to form ethyl bromide is carried out in a continuous reactor. The product stream is analyzed and found to contain 51.7 mole% C_2H_5Br and 17.3% HBr. The feed to the reactor contains only ethylene and hydrogen bromide. Calculate the fractional conversion of the limiting reactant and the percentage by which the other reactant is in excess. If the molar flow rate of the feed stream is 165 mol/s, what is the extent of reaction?




165 mol / s
x (mol C_2H_4 / mol)
$1 - x$ (mol HBr / mol)
$\dot{n}$ (mol / s)
0.310 mol C_2H_4 / mol
0.173 mol HBr / mol
0.517 mol C_2H_5Br / mol