

ChE445_HW2_Winter2020_Solution_and_Code

February 6, 2020

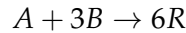
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Predicting conversion in non-ideal reactors (part 1)

Q1. Again review of 345: build a stoichiometric table. 40 pts

Consider a gaseous feed: $C_{A0} = 100 \text{ mol/L}$, $C_{B0} = 200 \text{ mol/L}$, $C_{inerts,0} = 100 \text{ mol/L}$ to a steady-state isothermal isobaric ideal PFR. At the reactor exit $C_A = 40 \text{ mol/L}$.

The gas-phase reaction is:

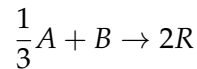


Find X_B and X_A . (Use any method and any approach to build a stoichiometric table). (Hint: these conversions are connected via exit flow rates)

Find a limiting reactant (LR) in $A + 3B \rightarrow 6R$

$$\frac{A}{B} = \frac{1 \text{ mol}}{2 \text{ mol}}$$

So B is the limiting reactant, this means that there is not enough B to convert all A . Therefore we can rewrite the reaction to have, 1 as the coefficient for the LR.



Stoichiometric table where $X = X_B$, $X = \frac{F_{B0} - F_B}{F_{B0}}$

Species	Initial	Change	Final
A	$F_{A0} = \frac{1}{2}F_{B0}$	$-\frac{1}{3}F_{B0}X$	$F_A = F_{B0}(\frac{1}{2} - \frac{1}{3}X)$
B	F_{B0}	$-F_{B0}X$	$F_B = F_{B0}(1 - X)$
R	0	$2F_{B0}X$	$F_C = 2F_{B0}X$
inert	$F_{I0} = \frac{1}{2}F_{B0}$	0	$F_I = \frac{1}{2}F_{B0}$
Total	$F_{T0} = 2F_{B0}$	$\frac{2}{3}F_{B0}X$	$2F_{B0}(1 + \frac{1}{3}X)$

$$C_A = \frac{F_A}{Q}$$

$$Q = \frac{Q_0}{F_{T0}} F_T \quad \text{at} \quad P, T = \text{CTE}$$

$$C_A = \frac{F_{B0}(\frac{1}{2} - \frac{1}{3}X)2F_{B0}}{Q_0 2F_{B0}(1 + \frac{1}{3}X)} = C_{B0} \frac{\frac{1}{2} - \frac{1}{3}X}{1 + \frac{1}{3}X} = 200 \left[\frac{\text{mol}}{\text{L}} \right] = 40 \frac{\text{mol}}{\text{L}}$$