ChE445_HW2_Winter2020_Solution_and_Code

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

The gas-phase reaction is:

$$A + 3B \rightarrow 6R$$

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 $A + 3B \rightarrow 6R$

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

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.

$$\frac{1}{3}A + B \rightarrow 2R$$

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	$F_{T0} = 2F_{B0}$	$\frac{2}{3}F_{B0}X$	$2F_{B0}(1 + \frac{1}{3}X)$

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

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

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