CRE—Spring 2020—Homework 2 Solutions

PROBLEM #1

a. LIQUID PHASE

$$A + 2B \longrightarrow C + D$$

$$r = kC_A C_B$$

$$C_A = C_{A0}(1 - X_A) \qquad C_C = C_{A0} X_A$$

$$C_B = C_{A0}(2 - 2X_A) \qquad C_D = C_{A0} X_A$$

$$\Theta_B = \frac{F_{B0}}{F_{A0}} = \frac{2}{1} = 2$$

$$V = \frac{F_{A0} X_A}{k C_A C_B} = \frac{v_0 \cancel{C_{A0}} X_A}{k \cancel{C_{A0}}(1 - X_A) C_{A0}(2 - 2X_A)}$$

$v_0 = 2\,L/min$ $\quad k = 0.1/(min \cdot M)$ $\quad C_{A0} = 0.5\,M$

$X_A = 0.9$

SUBSTITUTE IN

$$V_{CSTR} = \frac{2\,L/min\,(0.9)}{\frac{0.1}{min \cdot M}(1 - 0.9)(0.5M)(2 - 2(0.9))}$$

$$\boxed{V_{CSTR} = 1800\,L}$$

$$V_{PFR} = F_{A0}\int_0^{X_A} \frac{dX_A}{-r_A} = \cancel{C_{A0}} v_0 \int_0^{X_A} \frac{dX_A}{k C_{A0}^{\cancel{2}}(1-X_A)(2-2X_A)}$$

INTEGRATE NUMERICALLY WITH PYTHON...

$$\boxed{V_{PFR} = 180L}$$

b. GAS PHASE REACTION

$v \neq v_0 \longrightarrow$ FIND ϵ

$$\epsilon = \delta y_{A0} = (1+1-2-1)\left(\frac{1}{3}\right) = \frac{-1}{3}$$

$$C_A = \frac{C_{A0}(1-X_A)}{1-\frac{1}{3}X_A} \qquad C_B = \frac{C_{A0}(2-2X_A)}{1-\frac{1}{3}X_A}$$

$$C_C = \frac{C_{A0}X_A}{1-\frac{1}{3}X_A} \qquad C_D = \frac{C_{A0}X_A}{1-\frac{1}{3}X_A}$$

$$V_{CSTR} = \frac{F_{A0}X_A}{-r_A} = \frac{F_{A0}X_A}{kC_AC_B}$$

$$V_{CSTR} = \frac{v_0 C_{A0} X_A}{\frac{k C_{A0}(1-X_A) C_{A0}(2-2X_A)}{\left(1-\frac{1}{3}X_A\right)^2}}$$

SUBSTITUTE IN...

$$\boxed{V_{CSTR} = 882L}$$

$$V_{PFR} = F_{A0}\int_0^{X_A} \frac{dX_A}{-r_A}$$

$$V_{PFR} = \cancel{C_{A0}}\, v_0 \int_0^{0.9} \frac{dX_A\left(1-\frac{1}{3}X_A\right)^2}{k C_{A0}^{\cancel{2}}(1-X_A)(2-2X_A)}$$

SOLVE NUMERICALLY . . .

$$\boxed{V_{PFR} = 102\,L}$$

c. THE VOLUMES IN PART B ARE SMALLER BECAUSE THE VOLUMETRIC FLOW RATES ARE SMALLER AND CONCENTRATION INCREASES. WHEN CONCENTRATION INCREASES, THE RATE INCREASES FOR + ORDER KINETICS AS IN THIS SITUATION. FASTER RATES LEAD TO SMALLER VOLUMES NEEDED FOR THE SAME CONVERSION.

Problem #2

$$A + B \longrightarrow C + D$$

NEED TO PLOT $\frac{1}{-r_A}$ VS. X

a. CSTR Volume

$$F_B = F_{B0}(1-X)$$

$$V_{CSTR} = \frac{F_{B0} - F_B}{-r_B} = \frac{F_{B0} - F_{B0}(1-X)}{-r_B} = \frac{F_{B0}X}{-r_B}$$

FROM THE CHART, WHEN $X = 0.6$ $\quad -r_B = 10 \frac{mol}{L \cdot MIN}$

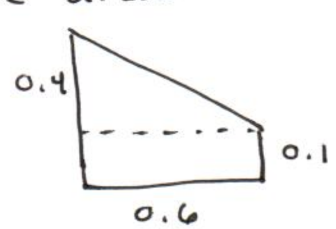
$$F_{B0} = 0.25\,(4\ mol/s) = 1\ mol/s$$

$$V_{CSTR} = \frac{(1\ mol/s)\left(\frac{60\,s}{min}\right)(0.6)}{10\ \frac{mol}{L \cdot min}} = 3.6\ L$$

b. PFR volume

$$V_{PFR} = F_{B0}\int^{X} \frac{dX}{-r_B} = \left(\frac{1\,mol}{s}\right)\left(\frac{60\,s}{MIN}\right) \cdot \left(\text{area under the curve}\right)$$

Curve area



$$0.06 + \tfrac{1}{2}(0.6 \cdot 0.4)$$

$$0.06 + 0.12$$

$$V_{PFR} = (60\,mol \cdot min^{-1})(0.18\ mol^{-1}\,dm^{3}\,MIN)$$

$$V_{PFR} = 10.8\,L$$

b. From part A, a 10.8L PFR leads to

$X_1 = 0.6$

CSTR: $F_B = F_{B0}(1-X_2)$

total conversion over both reactors

CSTR Design EQUATION

$$V_{CSTR} = \frac{F_{B0}(X_2 - X_1)}{-r_B|_{X_2}}$$

$$\frac{V}{F_{B0}} = \frac{3.6L}{60\,mol/min} = \frac{X_2 - 0.6}{-r_B|_{X_2}} = 0.06$$

DEFINE THE LINE FROM $X=0.7$ TO $X=0.9$

$$y = mx + b$$

$$m = \frac{\Delta y}{\Delta x} = \frac{0.3-0.1}{0.9-0.7} = 1$$

$$y = mx + b$$
$$0.1 = 1(0.7) + b$$
$$b = 0.6$$

$$\frac{-1}{r_B} = x - 0.6$$

At $x = 0.84$, $\frac{-1}{r_B} = 0.84 - 0.6 = 0.24$

$$X_2 - 0.6 = 0.24$$

$X_2 = 0.84$ by trial + error

c. From Part A, $X_1 = 0.6$

$$V_{PFR} = F_{A0} \int_{0.6}^{X_2} dX / -r_B$$

At $X_2 = 0.84$, the area under the curve is

$$y = \frac{-1}{r_B} = (1)(0.84) - 0.6$$

Total Area:

$$(0.1)(0.1) + (0.1)(0.14) + \frac{1}{2}(0.14)(0.14) = 0.0338$$

$$V_{PFR} = \left(60 \frac{mol}{min}\right)\left(0.0338 \frac{L}{mol\ min}\right)$$

$$V_{PFR} = 2.03\ L$$

d. Yes from $0.6 < X < 0.7$, the rate is independent of conversion

Thus for a feed $X = 0.6$ and an exit conversion $= 0.7$, the PFRs + CSTRs will have the same volumes.

e. CSTR to $X = 0.7$

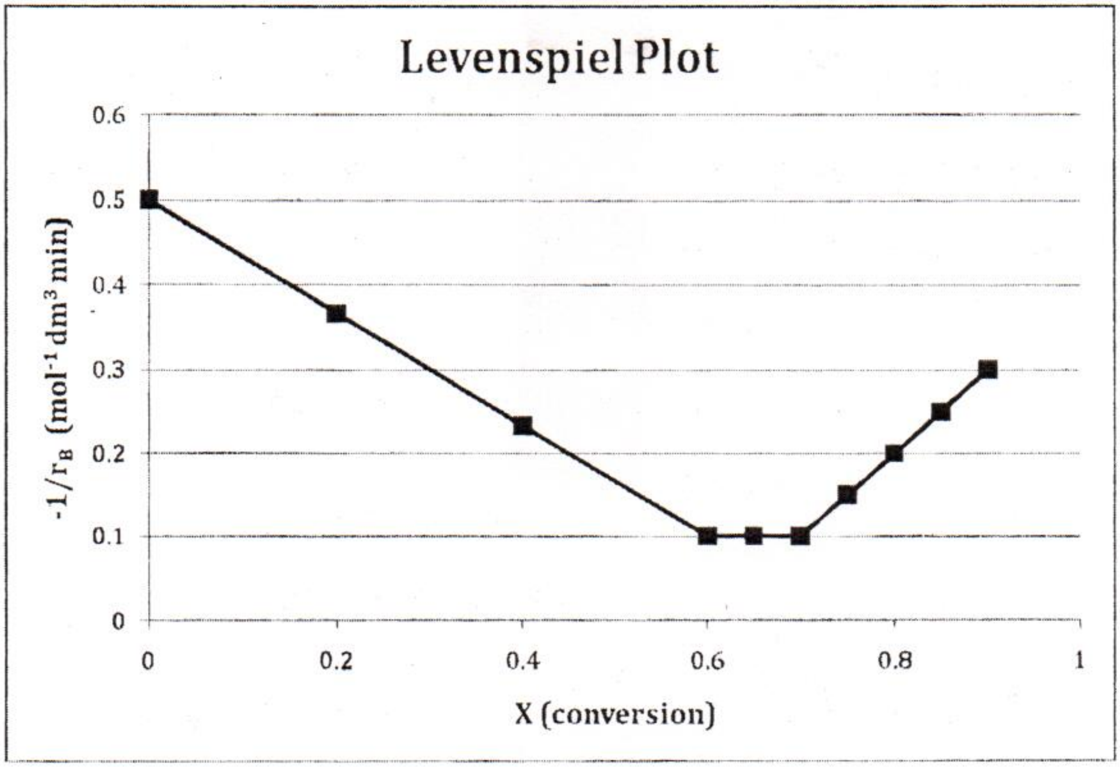
PFR to $X = 0.85$

or

CSTR to $X = 0.6$

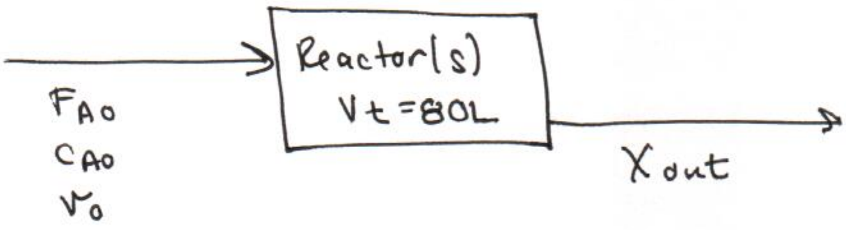
PFR or CSTR $X = 0.6$ to $X = 0.7$

PFR $X > 0.7$



Levenspiel Plot
0.6
0.5
0.4
0.3
0.2
0.1
0
$-1/r_B$ (mol^{-1} dm^3 min)
0
0.2
0.4
0.6
0.8
1
X (conversion)

Problem 3



CALCULATE INLET FROM COWS' RATE OF GRASS CONSUMPTION

$$\frac{170 \text{ lbs grass}}{8 \text{ hr}}\left(\frac{.105 \text{ lbs cellulose}}{1 \text{ lbs grass}}\right)\left(\frac{453.6 g}{\text{lbs}}\right)\left(\frac{\text{mol}}{162 g}\right)$$

$$= \frac{6.25 \text{ mol cellulose}}{\text{hr}} = F_{A0}$$

THE volumetric flow rate is calculated from the bulk density of grass

$$\frac{170 \text{ lbs grass}}{8 \text{ hr}}\left(\frac{453.6 g}{\text{lbs}}\right)\left(\frac{cm^3}{1.11 g}\right)\left(\frac{1 L}{1000 cm^3}\right) = 8.7 \frac{L}{hr}$$

$$C_{A0} = \frac{F_{A0}}{v_0} = \frac{\frac{6.25 \text{ mol}}{hr}}{8.7 \frac{L}{hr}} = 0.72 \frac{mol}{L}$$

THE DESIGN EQN FOR ALL 4 CSTRs is:

$$V = \frac{F_{A0}(X_{out} - X_{in})}{(-r_A)_{out}} = \frac{F_{A0}(X_{out} - X_{in})}{\left(\frac{k_{max} C_A}{K_M + C_A}\right)_{out}}$$

$$V = \frac{F_{A0}\left(X_{out} - X_{IN}\right)}{\dfrac{k_{MAX} C_{A0}\left(1 - X_{out}\right)}{K_M + C_{A0}\left(1 - X_{out}\right)}}$$

THIS EQN CAN BE SOLVED FOR X_{OUT} USING A NON-LINEAR EQUATION SOLVER FOR ALL 4 CSTRS.

THE CALCULATED CONVERSIONS FOR THE 4 CSTRS ARE:

$X_{out,1} = 0.307$

$X_{out,2} = 0.522$

$X_{out,3} = 0.671$

$X_{out,4} = 0.774$ ← ONLY NEED THIS ANSWER.

3b. DESIGN EQUATION FOR CSTR:

$$V = \frac{F_{A0}\left(X_{out} - \cancel{X_{IN}}^{\,0}\right)}{\dfrac{k_{MAX} C_{A0}\left(1 - X_{out}\right)}{K_M + C_{A0}\left(1 - X_{out}\right)}} = 80L = \frac{6.25 \frac{mol}{L}\left(X_{out}\right)}{\dfrac{2.8 \frac{mol}{L \cdot hr}\left(0.72 \frac{mol}{L}\right)\left(1 - X_{out}\right)}{14 \frac{mol}{L} + 0.72 \frac{mol}{L}\left(1 - X_{out}\right)}}$$

$$X_{out} = 0.644$$

3c. THE DESIGN EQN. FOR A PFR IS:

$$V = F_{A0}\int_{\cancel{X_{IN}}\,0}^{X_{out}} \frac{dX}{-r_A} = F_{A0}\int_0^{X_{out}} \frac{K_M + C_A}{k_{MAX} C_A}\, dX$$

$$V = F_{A0}\int_0^{X_{out}} \frac{K_M + C_{A0}\left(1 - X_{out}\right)}{k_{MAX} C_{A0}\left(1 - X_{out}\right)}\, dX_{out}$$

$$V = \frac{F_{A0}}{k_{MAX} C_{A0}}\int_0^{X_{out}} \frac{K_M + C_{A0} - C_{A0} X_{out}}{1 - X_{out}}\, dX_{out}$$

$$V = \frac{F_{A0}(K_M + C_{A0})}{k_{MAX} C_{A0}} \int_0^{X_{out}} \frac{1 - \frac{C_{A0}}{K_M + C_{A0}} X_{out}}{1 - X_{out}} \, dX_{out}$$

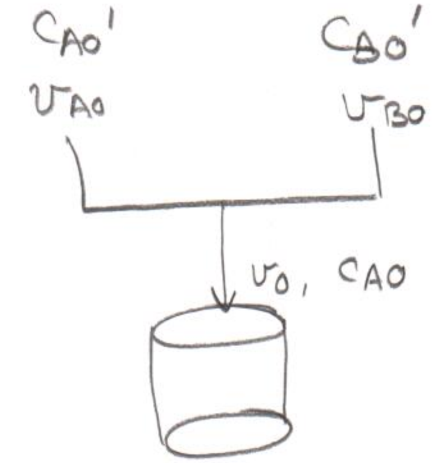
$$V = \frac{F_{A0}(K_M + C_{A0})}{k_{MAX} C_{A0}} \left[\left(1 - \frac{C_{A0}}{K_M + C_{A0}}\right) \ln\left(\frac{1}{1 - X_{out}}\right) + \frac{C_{A0}}{K_M + C_{A0}} X_{out} \right]$$

THIS EQUATION CAN BE SOLVED WITH AN NLE SOLVER.

$$\boxed{X_{out} = 0.834}$$

PROBLEM : 4

$2A + B \longrightarrow C$



$$v_0 = v_{AO} + v_{BO} = \frac{8\ L}{MIN}$$

$$C_{AO} = \frac{C_{AO}'\, v_{AO}}{v_A} = 1.25\ \frac{mol}{L}$$

FOR A CSTR

$$V_{CSTR} = \frac{F_{AO} X_A}{-r_A} = \frac{F_{AO} X_A}{k C_A^2}$$

$$V_{CSTR} = \frac{F_{AO} X_A}{k\, C_{AO}^2 (1-X_A)^2}$$

$$V_{CSTR} = \frac{\cancel{C_{AO}}\, v_0 X_A}{k\, C_{AO}^{\cancel{2}} (1-X_A)^2}$$

$$\frac{V_{CSTR}\, C_{AO}\, k}{v_0} = \frac{X_A}{(1-X_A)^2}$$

SOLVE FOR X_A $\longrightarrow$ $\boxed{X_A = 0.62}$

FOR A PFR

$$V_{PFR} = F_{AO} \int_0 \frac{dX_A}{k C_A^2} = \frac{F_{AO}}{k} \int \frac{dX_A}{C_{AO}^2 (1-X_A)^2}$$

$$\frac{V_{PFR}\, C_{AO}\, k}{v_0} = \frac{1}{1-X_A} - 1$$

$$1 - X_A = \frac{v_0}{V_{PFR}\, C_{AO}\, k}$$

$$\boxed{X_A = 0.87}$$

4b WE NEED TO IMPROVE THE CONVERSION OF THE 400L CSTR TO ACHIEVE 85% CONVERSION.

THE PARAMETERS THAT CAN BE CHANGED ARE v_{A0} + v_{B0}. LOWER v MEANS LESS DILUTED FEED, SO WE MUST LOWER THE FLOWRATES

ONE SOLUTION IS v_{A0} = 1 L/MIN

v_{B0} = 0.22 L/MIN.

Problem 5

$$2A \longrightarrow 3B + C$$

$$v = v_0 = \frac{7L}{hr} \qquad F_{A0} = C_{A0} v = (10\,mol/L)(7L/h) = 70 \frac{mol}{h}$$

$$F_A = F_{A0}(1-X) \quad X = 0.95$$

$$F_A = \frac{70\,mol}{h}(1-0.95) = 3.5 \frac{mol}{h}$$

FOR A CSTR

$$V = \frac{F_{A0} - F_A}{-r_A}$$

a) $-r_A = kC_A = (0.9h^{-1})(0.5\,MOL/L) = 0.45 \frac{mol}{L \cdot h}$

$$V_{CSTR} = \frac{70 \frac{mol}{h} - 3.5 \frac{Mol}{h}}{0.45 \frac{mol}{L \cdot h}} = \boxed{V = 148L}$$

b) $-r_A = kC_A^{-2} = \frac{0.6\,M^3/h}{\left(0.5 \frac{mol}{L}\right)^2} = 2.4 \frac{mol}{L \cdot hr}$

$$V_{CSTR} = \frac{70 \frac{mol}{h} - 3.5 \frac{mol}{h}}{2.4 \frac{mol}{L \cdot h}} = \boxed{28L}$$

c) $-r_A = k = 0.4 \frac{mol}{L \cdot h}$

$$V_{CSTR} = \frac{70 \frac{mol}{h} - 3.5 \frac{mol}{h}}{0.4 \frac{mol}{L \cdot hr}} = \boxed{166L}$$

PFR $\frac{dF_A}{dV} = r_A$

a. $r_A = -kc_A = \frac{-k F_A}{v}$

$$\int_{F_{A0}}^{F_A} \frac{dF_A}{F_A} = \frac{-k}{v} \int_0^V dV$$

$$\ln|F_A| \Big|_{F_{A0}}^{F_A} = \frac{-k}{v} V$$

$$V_{PFR} = \ln\left(\frac{3.5 \text{ mol/h}}{70 \text{ mol/h}}\right)\left(\frac{-7 \text{ L/h}}{0.9/\text{h}}\right) = \boxed{23.3 \text{ L}}$$

b. $r_A = \frac{-k}{c_A^2} = \frac{-k v^2}{F_A^2}$

$$\int_{F_{A0}}^{F_A} F_A^2 \, dF_A = -k v^2 \int_0^V dV$$

$$\frac{F_A^3}{3} \Big|_{F_{A0}}^{F_A} = -k v^2 V$$

$$V_{PFR} = \frac{(3.5 \text{ mol/h})^3 - (70 \text{ mol/h})^3}{3(-0.6 \text{ M}^3/\text{h})(7 \text{ L/h})}$$

$$\boxed{V_{PFR} = \cancel{2.72 \times 10^4} \; 3.89 \times 10^3 \text{ L}}$$

c. $r_A = -k$ $\int_{F_{A0}}^{F_A} dF_A = -k \int_0^V dV$

$$V_{PFR} = \frac{F_A - F_{A0}}{-k} = \boxed{166 \text{ L}}$$

5d.

a $V_{PFR} < V_{CSTR}$

$$(148L - 23.3L)\left(\frac{\$750}{L}\right) = \$93.5K$$

Savings for PFR

b $V_{PFR} > V_{CSTR}$

$$(\cancel{2.72\times10^4}\ 3.89\times10^3\,L - 28L)\left(\frac{\$750}{L}\right) = \$2.9\text{ million}$$

Savings for CSTR

c. $V_{PFR} = V_{CSTR}$ NO COST DIFFERENCE