Assignment 1 - solutions

1. The exothermic reaction of stillbene (A) to form the economically important trospophene (B) and methane (C),

$$A \rightarrow B + C$$

was carried out adiabatically and the following data recorded:

X	0	0.2	0.4	0.45	0.5	0.6	0.8	0.9
$-r_A$ mol/(L.min)	1.0	1.67	5.0	5.0	5.0	5.0	1.25	0.91

The entering molar flow rate of A was 300 mol/min.

(a) What are the PFR and CSTR volumes necessary to achieve 40% conversion?
CSTR: $V = F_{A0}X/(-r_A)$ = 300 * 0.4/5 = 24 liter. [1 Mark]
PFR: $V = F_{A0}\int_0^X \frac{dX}{-r_A}$ = 300* [0.2*0.4 + 0.5*0.4*0.8] = 72 liter. [1 Mark]

(b) Over what range of conversions would the CSTR and PFR reactor volumes be identical? $X \in [0.4 - 0.6]$ [1 Mark]

(c) What is the maximum conversion that can be achieved in a 105L CSTR?

$$\frac{X}{-r_A} = \frac{V}{F_{A0}} = 0.35$$

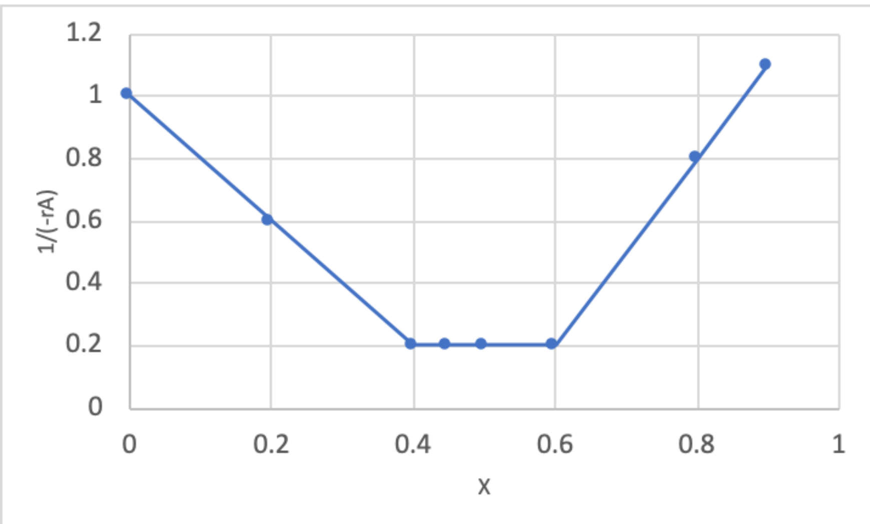
From the reaction rate plot (see below), at X = 0.7, $\frac{X}{-r_A} = 0.35$. So maximum conversion possible is X = 0.7. [1 Mark]

(d) What conversion can be achieved if a 72L PFR is followed in series by a 24L CSTR?
X_1 = 0.4 (from a)
$\frac{X_2 - X_1}{-r_A} = \frac{V}{F_{A0}} = \frac{24}{F_{A0}} = 0.08.$ From interpolation, $X_2 \approx 0.64$. [1 Mark]

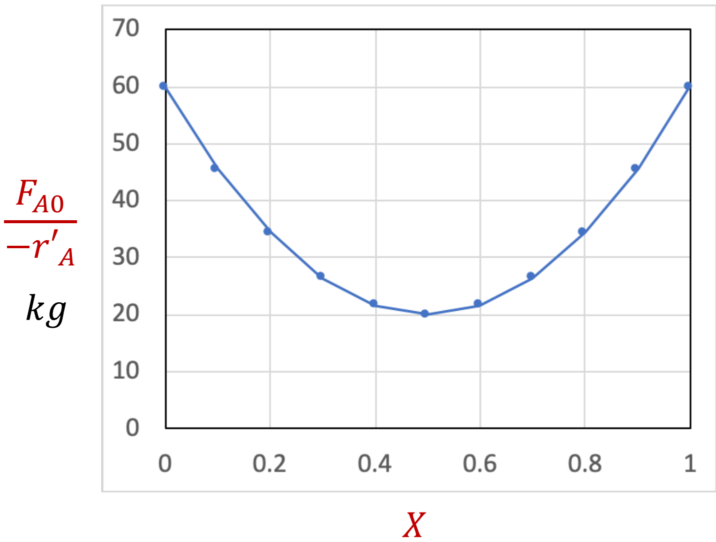
(e) What conversion can be achieved if a 24L CSTR is followed in a series by a 72L PFR?
X_1 = 0.4 (from a)

$$\frac{V}{F_{A0}} = \int_{X_1}^{X_2} \frac{dX}{-r_A} = 0.24$$

From interpolation, $X_2 \approx 0.9$ to 0.91. [1 Mark]



2. The curve shown below is typical of a gas-solid catalytic exothermic reaction carried out adiabatically.



The curve can be approximated to $\frac{F_{A0}}{-r_A'} = 20 + 160(X - 0.5)^2$. For F_{A0} = 2 mol/s,

(a) Assuming that you have a fluidized CSTR and a PBR containing equal weights of catalyst, how should they be arranged for this adiabatic reaction? Use the smallest amount of catalyst weight to achieve 80% conversion of A. [Total Marks = 6]

Clearly parallel arrangement can be ruled out because PBR will give low conversion if fresh feed is used (see the shape of the curve from X =0 to 0.5). [2 Marks for explicit calculation or for reasoning]

From the shape of the curve, minimum total weight of catalyst can be achieved by CSTR-PBR in series:
For equal weights of catalyst: $\frac{F_{A0}X_1}{-r'_A} = \int_{X_1}^{0.8} \frac{F_{A0}}{-r'_A} dX$
Since analytical expression for $\frac{F_{A0}}{-r_A'}$ is given, the above equation can be solved to yield, X_1 = 0.428 (or any value between 0.42 and 0.43 is acceptable.)

This corresponds to a total weight (W_{CSTR} + W_{PBR}) of **17.8 kg** [2 Marks]

It may be verified that PBR-CSTR in series will require higher weight of catalyst. [**2 Marks**]

(b) What is the catalyst weight necessary to achieve 80% conversion in a fluidized CSTR?
W_{CSTR} = 27.5 kg [1 Mark]

(c) What is the catalyst weight necessary to achieve 40% conversion in a fluidized CSTR?
W_{CSTR} = 8.6 kg [1 Mark]

(d) What is the catalyst weight necessary to achieve 80% conversion in a fluidized PBR?
W_{PBR} = 24.1 kg [1 Mark]

(e) What is the catalyst weight necessary to achieve 40% conversion in a fluidized PBR?
W_{PBR} = 14.7 kg [1 Mark]

Inference: For 40% conversion, the weights of catalyst required in CSTR and PBR are significantly different, but for 80% conversion, both reactors require almost similar weight of catalyst. It may be possible to find the conversion for which CSTR and PBR require equal weight of catalyst (See the figure below; X = 0.75 satisfies this condition). [If any student has done this analysis, which was not asked for, he/she will get a ☆]