HW # 2

1. General equation

$F_{in} - F_{out} + \text{Generation} = \cancel{\text{accumulation}}$

$\text{Generation} = (-r_A)\, \Delta V\, (1-\varepsilon)$

$F_{A,V} - F_{A,V+\Delta V} - r_A\, \Delta V\, (1-\varepsilon) = 0$

$$\Rightarrow \boxed{\frac{dF_A}{dV} = -r_A(1-\varepsilon)}$$

2. $F_i - F_{out} + G = \dfrac{dN_A}{dt}$

$F_i = 0$

$G_j = 2.5 \times 10^{-7}$ mole/m^2 s

$C_{0,\,stink} = 5 \times 10^{-3}$ mole/m^3

$\nu_0 = 0.1$ m^3/s

$F_{out} = \nu_0 C_{s,\,out}$

$V = 5 \times 8 \times 2.5 = 100$ m^3

$A = 5 \times 8$ m^2

(a) steady-state

$$\cancel{F_i} - F_{out} + G = \cancel{\frac{dN_A}{dt}}$$

$-\nu_0 C_{s,\,out} + G_j A = 0$

$-0.1 \times C_{s,\,out} + 2.5 \times 10^{-7} \times 40 = 0$

$\boxed{C_{s,\,out} = 10^{-4} \text{ mole/m}^3}$

(b) not steady state

$$\cancel{F_i} - F_{out} + G = \frac{dN_A}{dt}$$

$$-F_{out} + G = \frac{dC_S V}{dt}$$

$$\frac{-\nu_0 C_S + G_j A}{V} = \frac{dC_S}{dt}$$

$$-\frac{\nu_0}{V} dt = \frac{dC_S}{\left(C_S - \dfrac{G_j A}{\nu_0}\right)}$$

$$\int_0^{3600} (-10^{-4})dt = \int_{C_{S,0}}^{C_S} \frac{dC_S}{(C_S - 10^{-7})}$$

$\boxed{C_S = 2.34 \times 10^{-4} \text{ mole/m}^3}$

3. $A \rightarrow B$

$X = 0.99$

$F_{A0} = 5$ mol / h

$\nu_0 = 10$ dm^3 / h

$C_{A0} = 0.5$ mole / dm^3

For CSTR $V = \dfrac{F_{A0}X}{-r_A}$

For PFR $\dfrac{dF_A}{dV} = r_A$

$F_A = F_{A0}(1-X) \rightarrow dF_A = -F_{A0}dX$

$$F_{A0}\frac{dX}{dV} = -r_A$$

(a) $-r_A = k$ $k = 0.05$

0

For CSTR $V = \dfrac{5 \times 0.99}{0.05} = \boxed{99 dm^3}$

For PFR $5\int_0^{0.99} \dfrac{dX}{0.05} = \int dV$

$\boxed{V = 99 \text{ dm}^3}$

(b) $-r_A = kC_A$ $k = 0.0001 s^{-1}$

For CSTR $V = \dfrac{F_{A0}X}{-r_A} = \dfrac{F_{A0}X}{kC_A} = \dfrac{\nu_0 C_{A0}X}{kC_{A0}(1-X)} = \dfrac{\nu_0 X}{k(1-X)} = \boxed{2750 dm^3}$

$$\frac{dF_A}{dV} = -F_{A0}\frac{dX}{dV} = r_A = -kC_A$$

For PFR $\nu_0 C_{A0}\dfrac{dX}{dV} = kC_{A0}(1-X)$

$$\frac{\nu_0}{k}\int_0^{0.99} \frac{dX}{(1-X)} = \int dV$$

V=$\boxed{127.92 dm^3}$

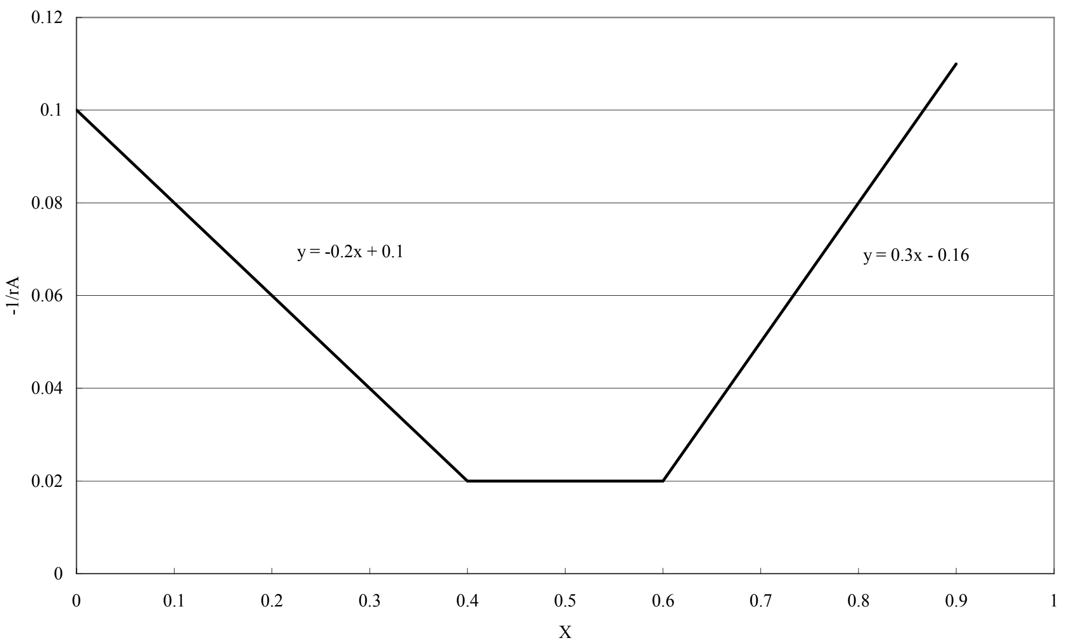
(c) $-r_A = kC_A^2$ $k = 3$ dm^3/mol h

For CSTR $V = \dfrac{F_{A0}X}{-r_A} = \dfrac{\nu_0 C_{A0}X}{kC_{A0}^2(1-X)^2} = \dfrac{\nu_0 X}{kC_{A0}(1-X)^2} = \boxed{66000 dm^3}$

For PFR
$$\frac{dF_A}{dV} = -F_{A0}\frac{dX}{dV} = r_A = -kC_A{}^2 = -kC_{A0}{}^2(1-X)^2$$
$$\frac{\nu_0}{kC_{A0}}\frac{dX}{(1-X)^2} = dV$$
$$\boxed{V = 660 dm^3}$$

4. (for 3rd edition)

X	0	0.2	0.4	0.6	0.8	0.9
r_A	10	16.67	50	50	12.5	90.9
$1/r_A$	0.1	0.06	0.02	0.02	0.8	0.11



(a)

$$V_{CSTR} = \frac{F_{A0}X}{-r_A} = \frac{300\times 0.4}{50} = \boxed{2.4\ \mathrm{dm}^3}$$

$$V_{PFR} = F_{A0}\int_0^X \frac{dX}{-r_A} = 300\times\frac{(0.1+0.02)}{2}\times 0.4 = \boxed{7.2\ \mathrm{dm}^3}$$

(b) Between 0.4 ~ 0.6, because the rate is constant over this conversion range.

(c) $V_{CSTR} = 10.5\ \mathrm{dm}^3$

$$= \frac{F_{A0}X}{-r_A} = 300\times\frac{X}{-r_A}$$

=> $\frac{X}{-r_A}$ =0.035

You can trial and error until $\frac{X}{-r_A}$ =0.035, or just calculate area from the plot.

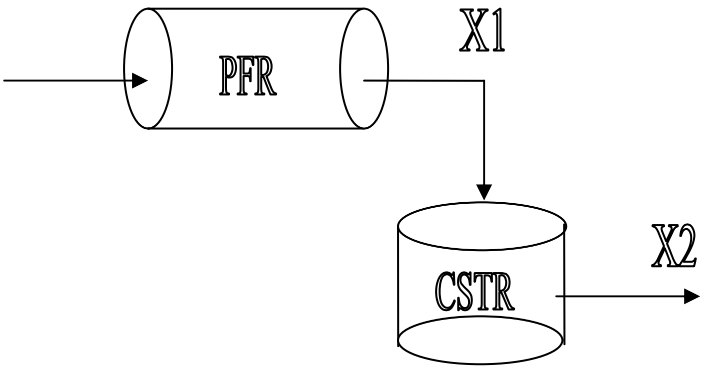
From X=0.4 V_1= 2.4

X=0.6 V_2 =3.6

10.5 = 300 X (0.3X-0.16)

Maximum conversion $\boxed{X = 0.7}$

(d)

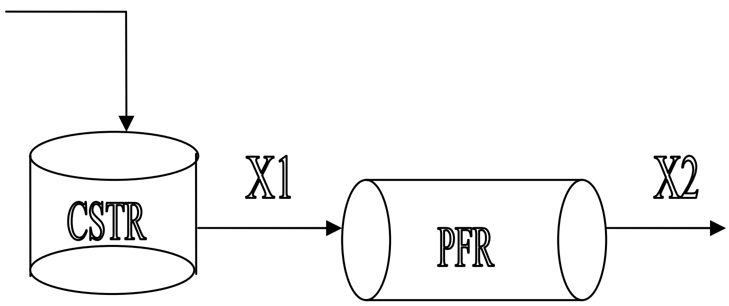


From part (a) we know X_1 = 0.4

V_{CSTR} = 2.4 = 300(X_2-0.4)(0.3X_2-0.16)

$\boxed{X= 0.64}$

(e)

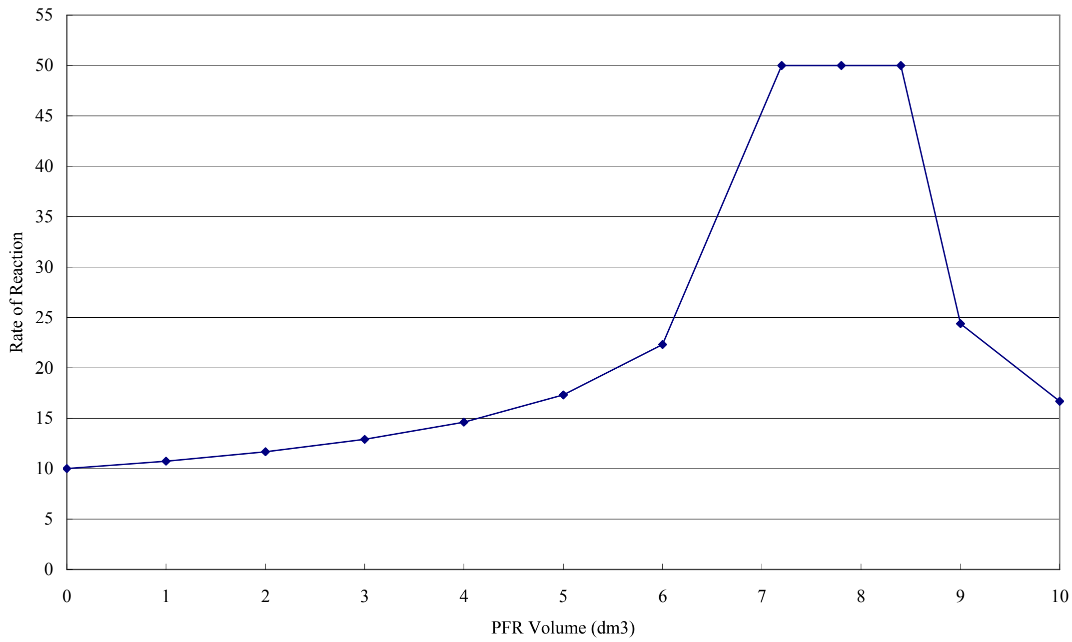


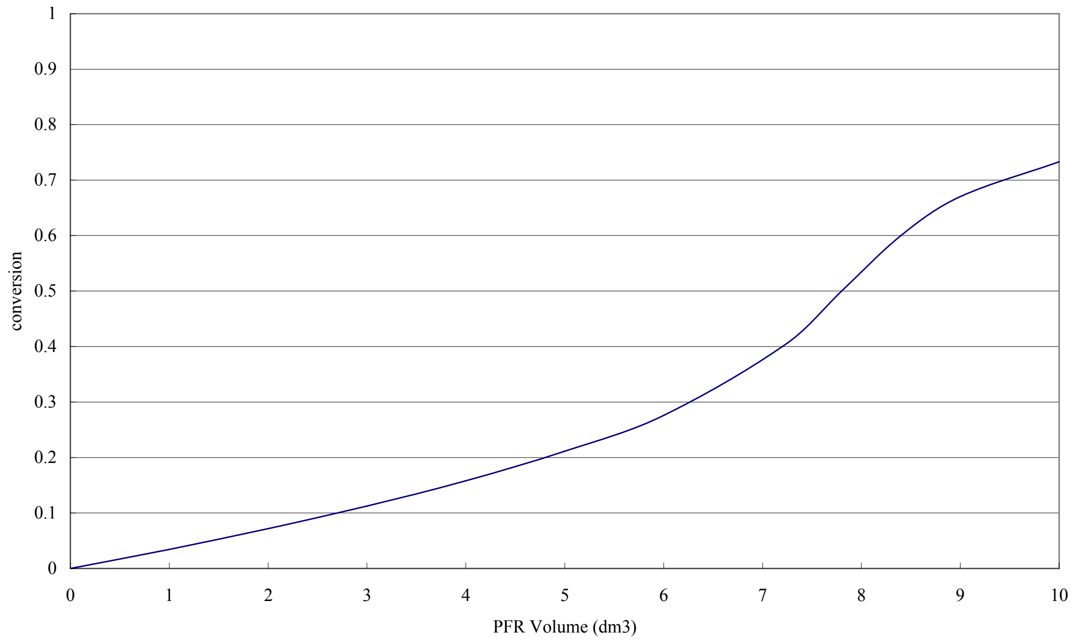
From part (a) we know X_1 = 0.4

$$V_{PFR} = 7.2 = F_{A0} \int_0^X \frac{dX}{-r_A} = 300 \int_{0.4}^{X2} \frac{dX}{-r_A} = 1.2 + 300 \int_{0.6}^{X2} (0.3X - 0.16)dX$$

$\boxed{X_2 = 0.905}$

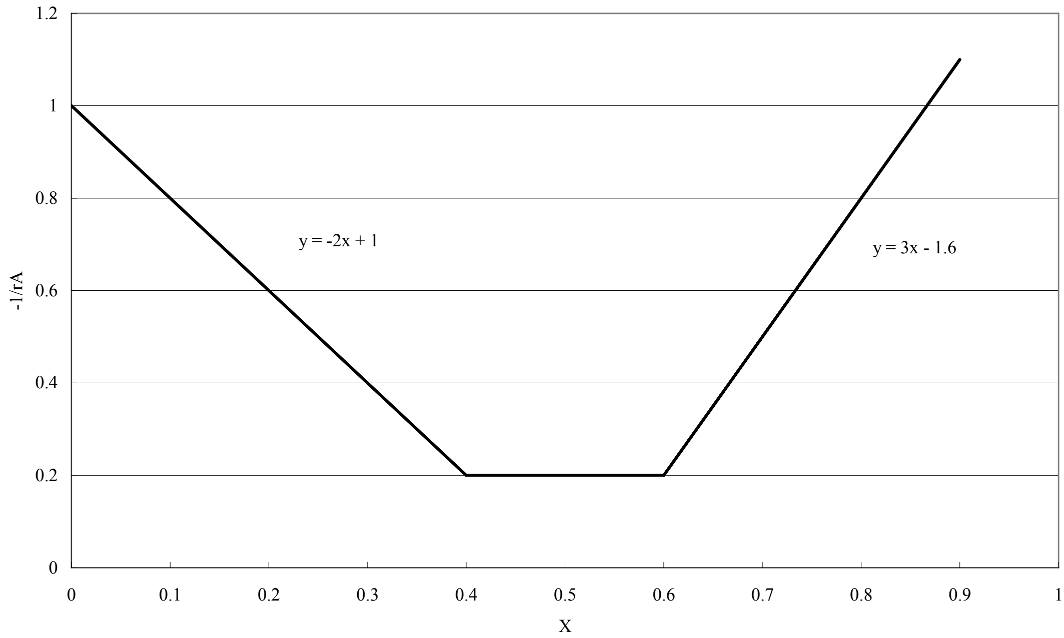
(f)





4. for 4th edition

X	0	0.2	0.4	0.6	0.8	0.9
r_A	1	1.67	5.0	5.0	1.25	0.91
$1/r_A$	1	0.6	0.2	0.2	0.8	1.1



(a)

$$V_{CSTR} = \frac{F_{A0}X}{-r_A} = \frac{300\times 0.4}{5} = \boxed{24\ dm^3}$$

$$V_{PFR} = F_{A0}\int_0^X \frac{dX}{-r_A} = 300\times\frac{(1+0.2)}{2}\times 0.4 = \boxed{72\ dm^3}$$

(b) Between 0.4 ~ 0.6, because the rate is constant over this conversion range.

(c) $V_{CSTR} = 10.5\ dm^3$

$$= \frac{F_{A0}X}{-r_A} = 300\times\frac{X}{-r_A}$$

$$\Rightarrow \frac{X}{-r_A} = 0.035$$

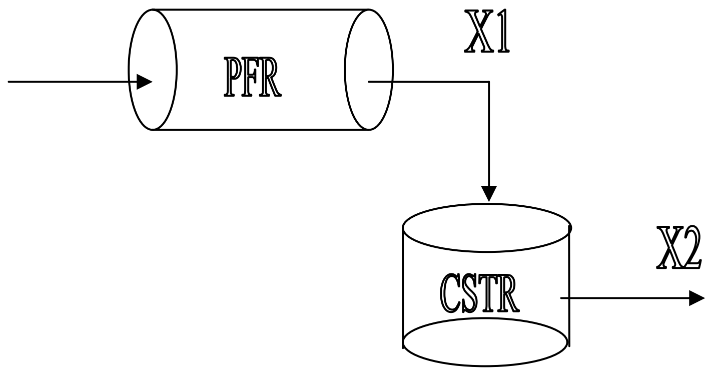
You can trial and error until $\frac{X}{-r_A}$ =0.035, or just calculate area from the plot.

From X=0.4 $\quad V_1 = 24$

10.5 = 300 X (-2X+1)

Maximum conversion $\boxed{X = 0.0378}$

(d)

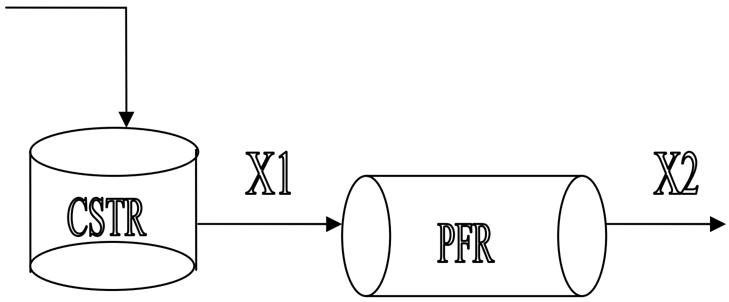


From part (a) we know $X_1 = 0.4$

$V_{CSTR} = 24 = 300(X_2-0.4)(3X_2-1.6)$

$\boxed{X = 0.64}$

(e)

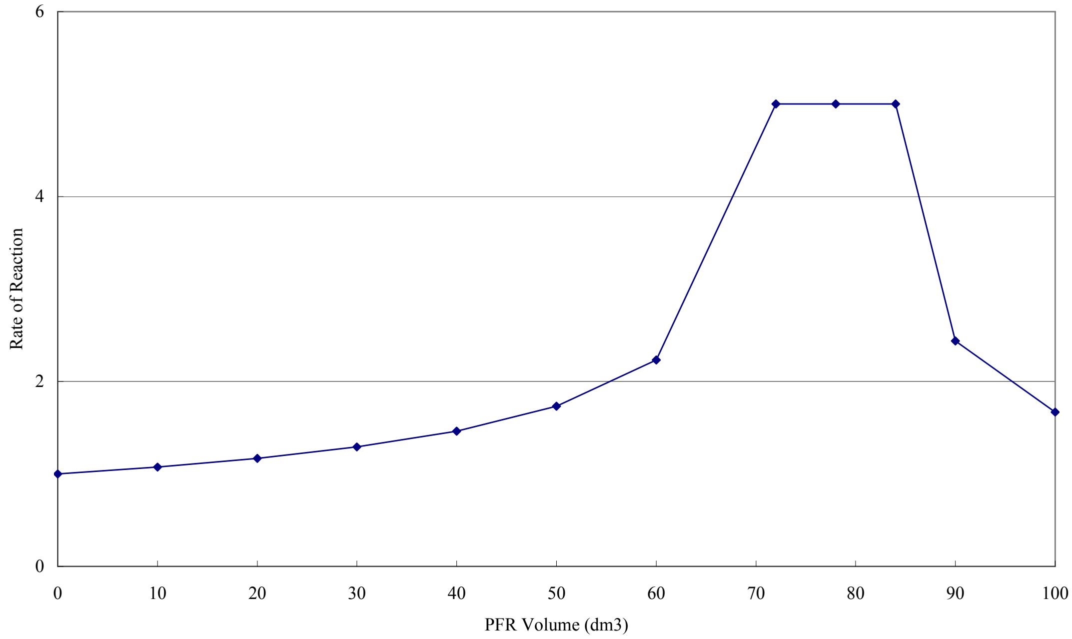


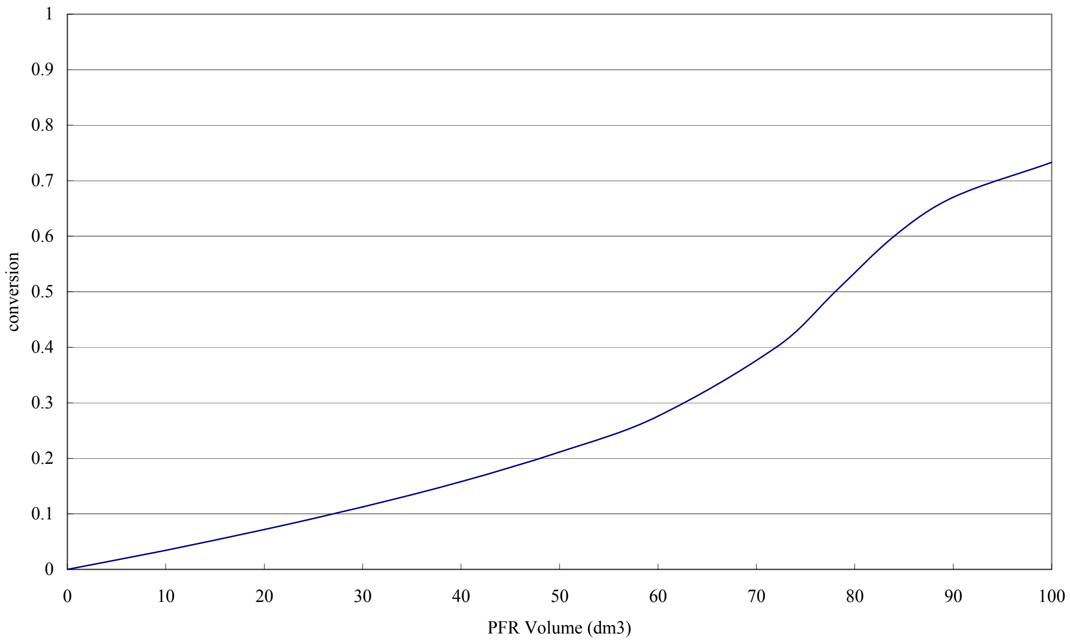
From part (a) we know $X_1 = 0.4$

$$V_{PFR} = 72 = F_{A0} \int_0^X \frac{dX}{-r_A} = 300 \int_{0.4}^{X2} \frac{dX}{-r_A} = 12 + 300 \int_{0.6}^{X2} (3X - 1.6)dX$$

$\boxed{X_2 = 0.905}$

(f)

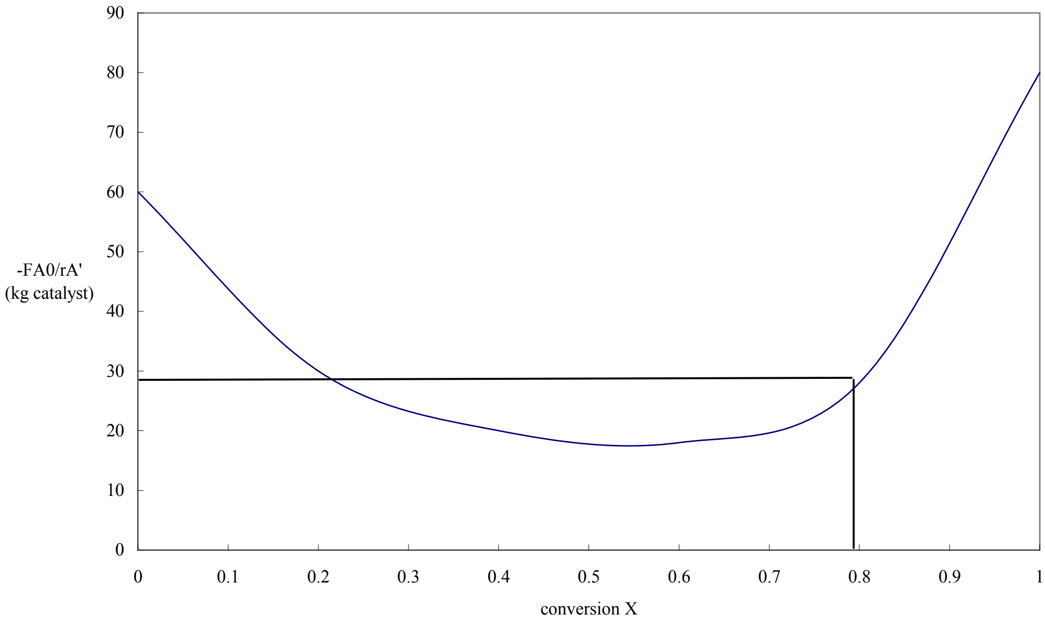

6
4
2
0
Rate of Reaction
0
10
20
30
40
50
60
70
80
90
100
PFR Volume (dm3)


1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
conversion
0
10
20
30
40
50
60
70
80
90
100
PFR Volume (dm3)

5.

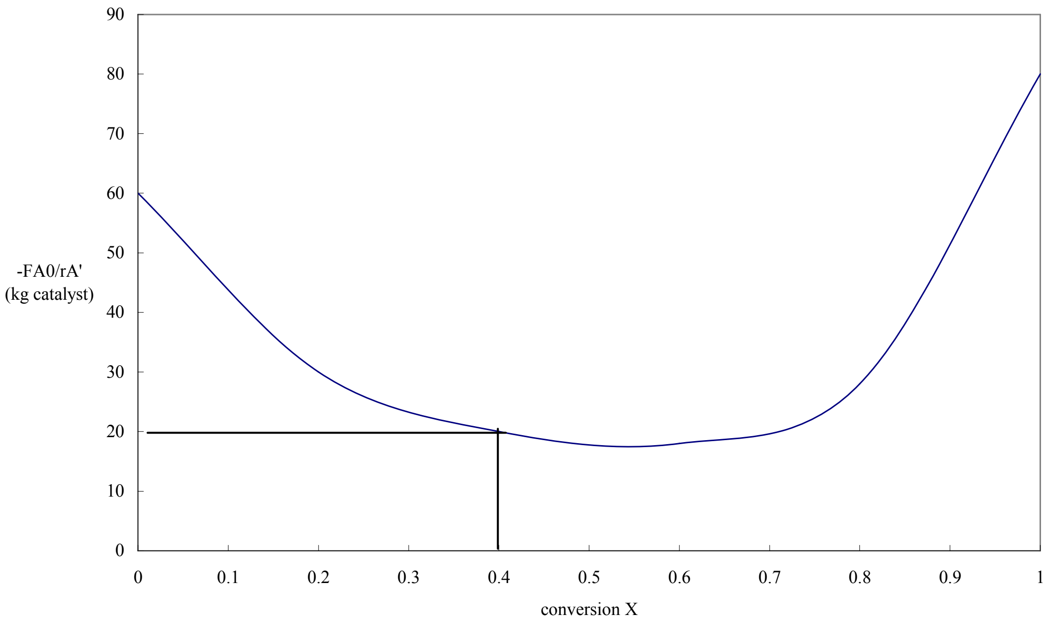
(a) CSTR is used before PFR.

(b) One can calculate the amount of catalyst needed to carry out the same reaction to 80 % conversion using a single CSTR by determining the area of the rectangle.



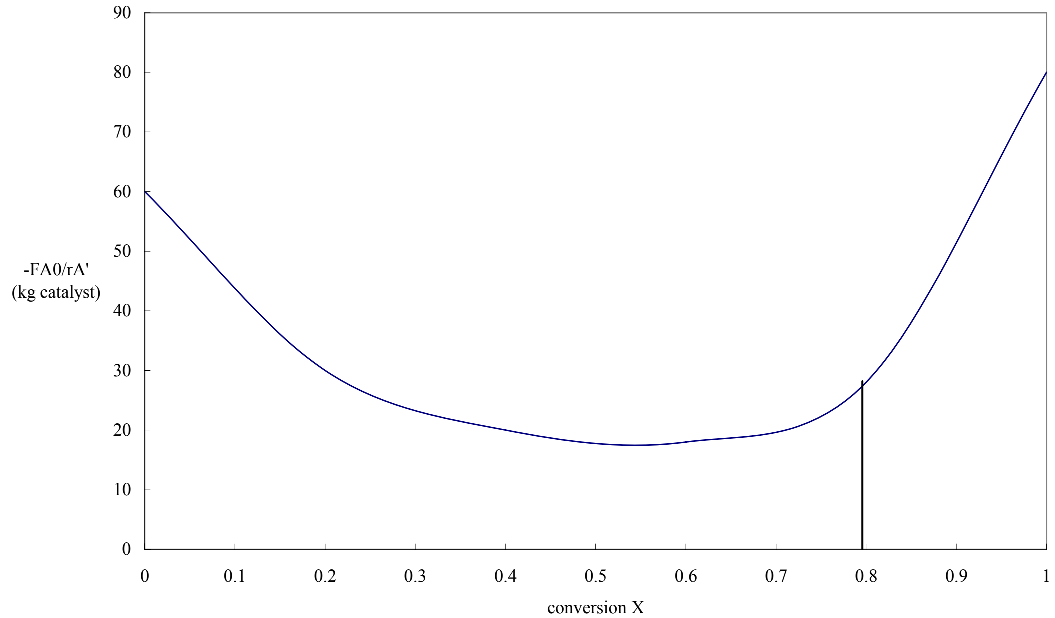
approximately $\boxed{\text{22.4 kg catalyst.}}$

(c) for 40 % conversion



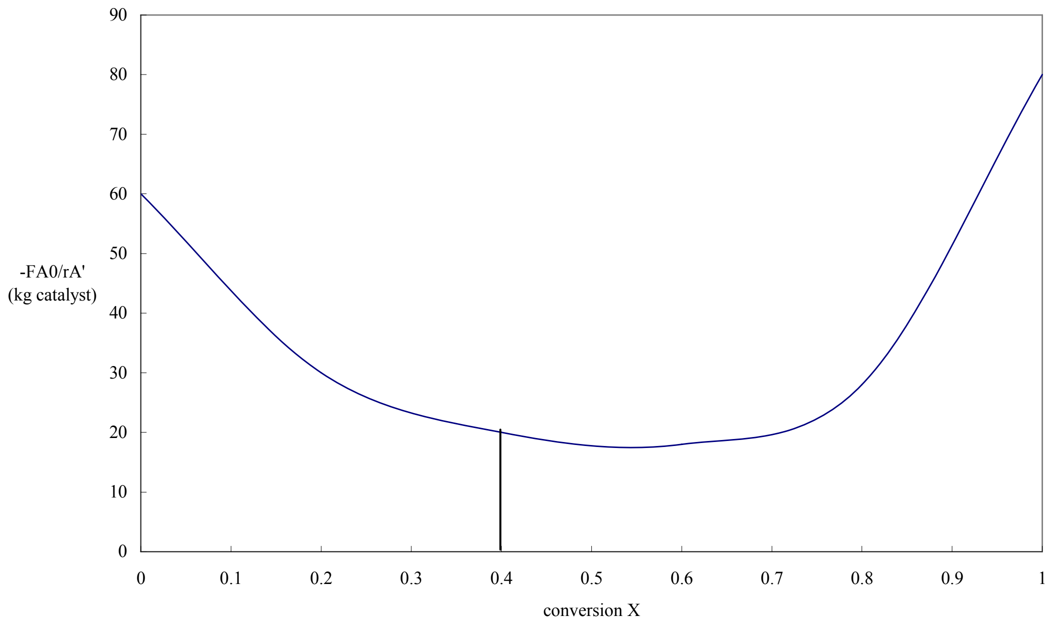
➔ $\boxed{\text{8 kg catalyst}}$

(d)



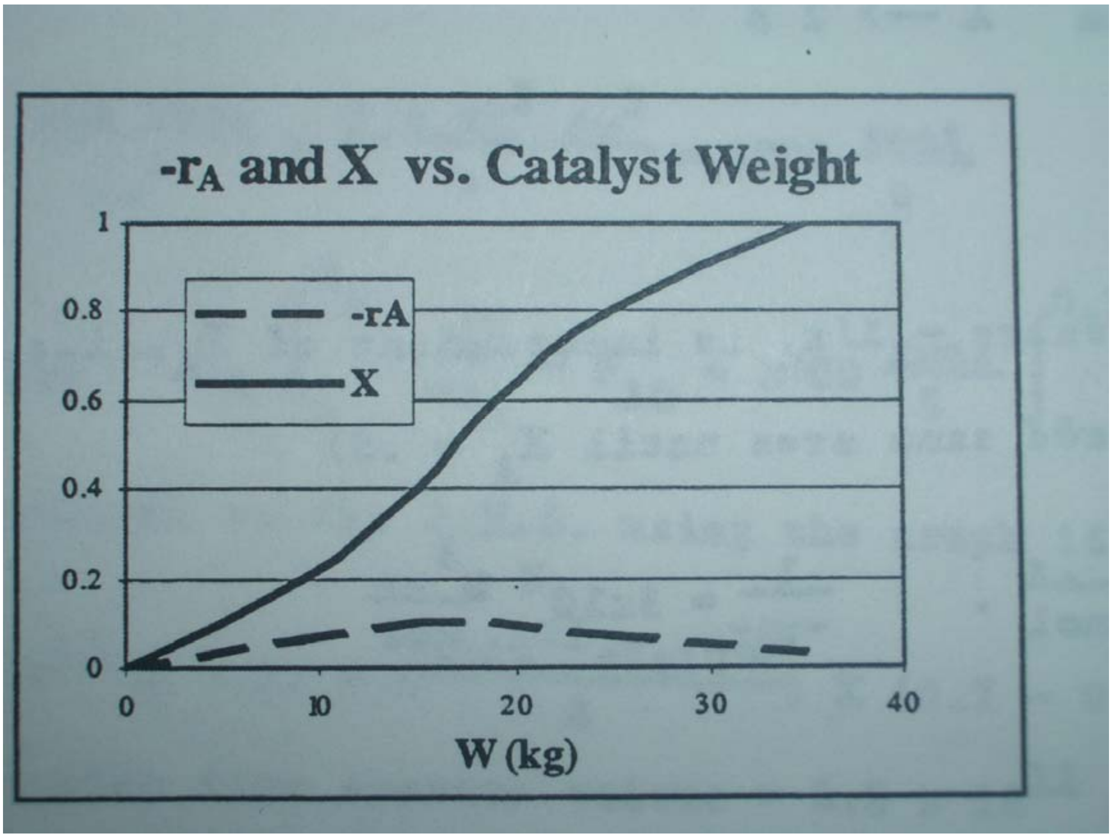
Calculate the area under the curve between 0 and 0.8. Approximately $\boxed{30\text{ kg}}$

(e)



Calculate the area under the curve between 0 and 0.4 Approximately $\boxed{15\text{ kg}}$

(f)



(g) For different ($-r_A$) vs. (X) curves, reactors should be arranged so that the smallest amount of catalyst is needed to give the maximum conversion. This can be done by minimizing the area that is occupied be a given reactor. One useful heuristic is that for curves with a negative slope, it is generally better to use a CSTR. Similarly, when the curve has a positive slope, it is generally better to use a PFR.