Sheet 2

Q1:

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05

a) use one of the integration formulas given in Appendix A.4 to determine the PER reactor volume necessary to achieve 80% conversion

b) If the initial volumetric flowrate and concentration are 2 dm3/s (0.002 m3/s), and 0.2 mol/dm3, respectively. calculate the space time and space velocity

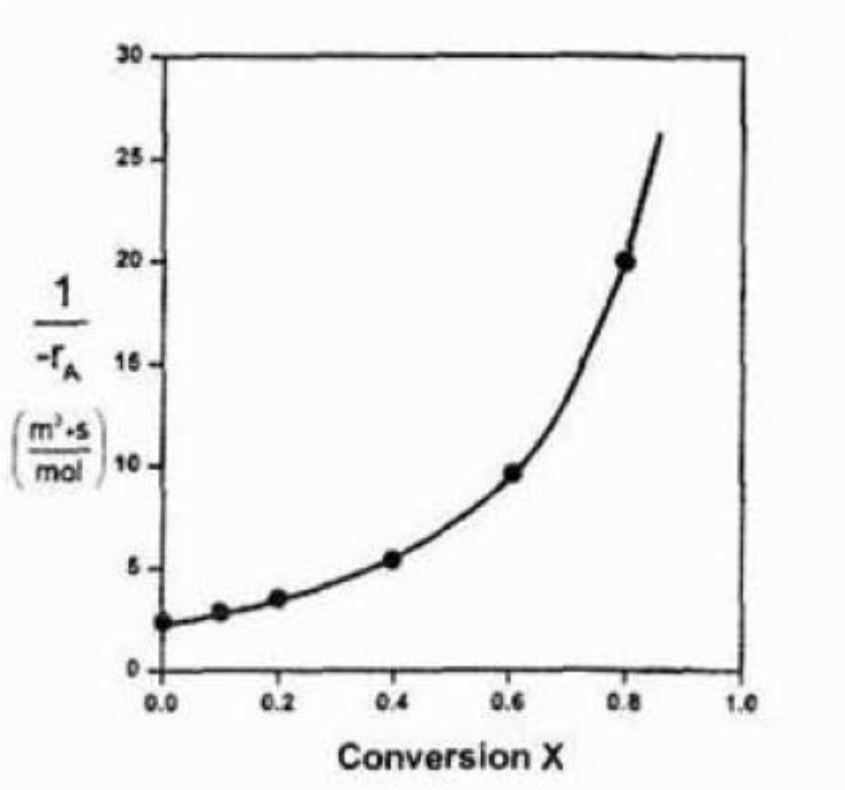
(Fogler book, example 2-3, page 50)

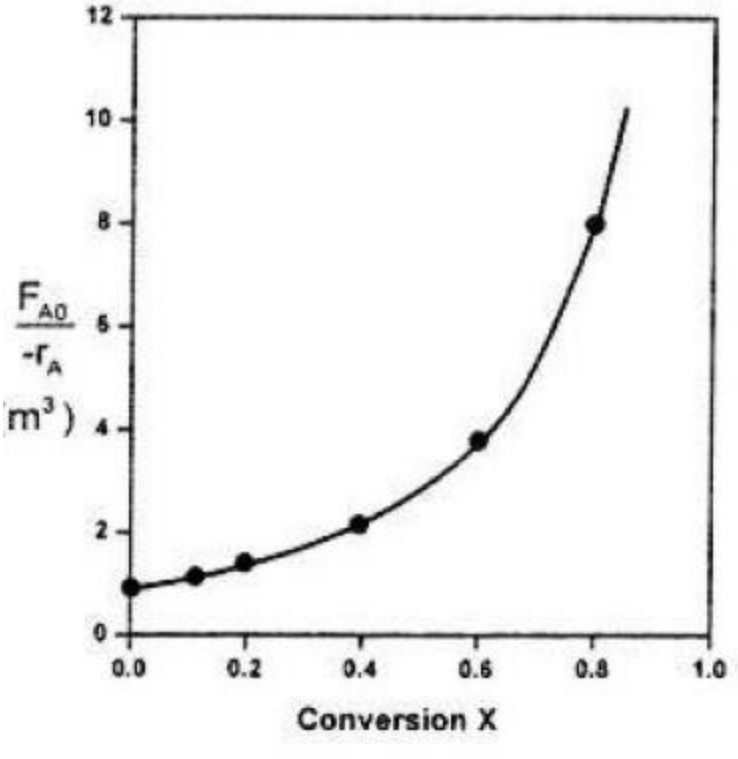
Q2: The space time required to achieve 80% conversion in a CSTR is 5 h. The entering volumetric flow rate and concentration of reactant A are 1 dm3/min and 2.5 molar, respectively. IF possible determine:

(1) the rate of reaction (-rA)
(2) the reactor volume (V)
(3) the exit concentration of A (CA)

ANS(solution manual, p2-4(e) , page 38)

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{mol}{m^3 \cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{m^3 \cdot s}{mol}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](m^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0





For CSTR:

$$V = \frac{F_{A0}X}{(-r_A)_{\text{exit}}}$$

$$V = \left[\frac{F_{A0}}{-r_A}\right]_{X=0.8} (0.8)$$

V = Levenspiel rectangle area = height × width

$$V = [8\ \text{m}^3][0.8] = 6.4\ \text{m}^3$$

$$V = 0.4\frac{\text{mol}}{\text{s}}\left(\frac{20\ \text{m}^3 \cdot \text{s}}{\text{mol}}\right)(0.8) = 6.4\ \text{m}^3$$

$$V = 6.4\ \text{m}^3 = 6400\ \text{dm}^3 = 6400 l$$

PFR

$$V = F_{A0}\int_0^{0.8} \frac{dX}{-r_A} = \int_0^{0.8} \frac{F_{A0}}{-r_A} dX$$

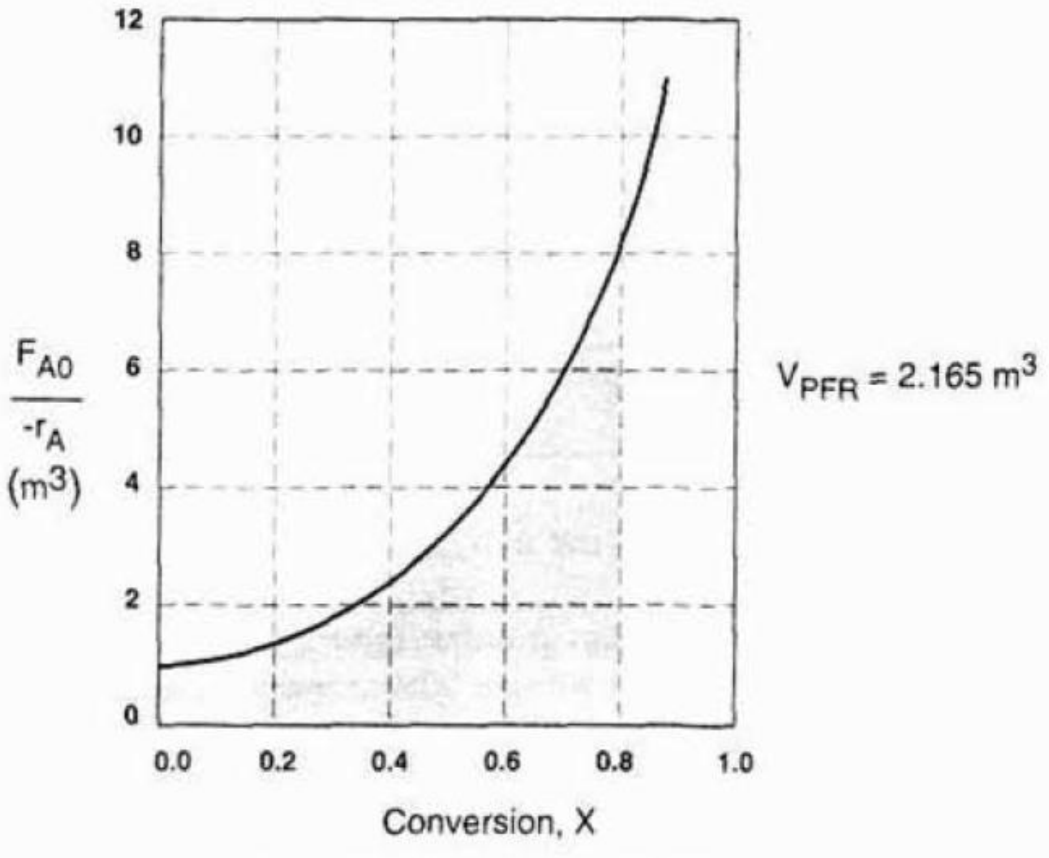
We shall use the *five point quadrature* formula (A-23) given in Appendix A.4 to numerically evaluate Equation (2-16). For the five-point formula with a final conversion of 0.8, gives for four equal segments between $X = 0$ and $X = 0.8$ with a segment length of $\Delta X = \frac{0.8}{4} = 0.2$. The function inside the integral is evaluated at $X = 0$, $X = 0.2$, $X = 0.4$, $X = 0.6$, and $X = 0.8$.

$$V = \frac{\Delta X}{3}\left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{2F_{A0}}{-r_A(X=0.4)} + \frac{4F_{A0}}{-r_A(X=0.6)} + \frac{F_{A0}}{-r_A(X=0.8)}\right]$$

Using values of $F_{A0}/(-r_A)$ in Table 2-3 yields

$$V = \left(\frac{0.2}{3}\right)[0.89 + 4(1.33) + 2(2.05) + 4(3.54) + 8.0]\text{dm}^3 = \left(\frac{0.2}{3}\right)(32.47\ \text{m}^3)$$

$$\boxed{V = 2.165\ \text{m}^3 = 2165\ \text{dm}^3}$$



product. For $X = 0.2$, we calculate the corresponding reactor volume using Simp son's rule (given in Appendix A.4 as Equation [A-21]) with $\Delta X = 0.1$ and the dat in rows 1 and 4 in Table 2-3.

$$V = F_{A0}\int_0^{0.2} \frac{dX}{-r_A} = \frac{\Delta X}{3}\left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.1)} + \frac{F_{A0}}{-r_A(X=0.2)}\right]$$

$$= \left[\frac{0.1}{3}[0.89 + 4(1.08) + 1.33]\right]\text{m}^3 = \frac{0.1}{3}(6.54\ \text{m}^3) = 0.218\ \text{m}^3 = 218\ \text{dm}^3$$

$$= 218\ \text{dm}^3$$

For $X = 0.4$, we can again use Simpson's rule with $\Delta X = 0.2$ to find the reactoı volume necessary for a conversion of 40%.

$$V = \frac{\Delta X}{3}\left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{F_{A0}}{-r_A(X=0.4)}\right]$$

$$V = \frac{\Delta X}{3}\left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{F_{A0}}{-r_A(X=0.4)}\right]$$

$$= \left[\frac{0.2}{3}[0.89 + 4(1.33) + 2.05]\right]\text{m}^3 = 0.551\ \text{m}^3$$

$$= 551\ \text{dm}^3$$

X	0	0.2	0.4	0.6	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.30	0.195	0.113	0.05
V (dm^3)	0	218	551	1093	2165

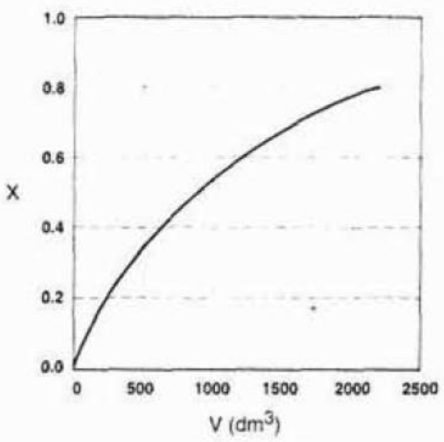


Figure E2-3.2(a) Conversion profile.

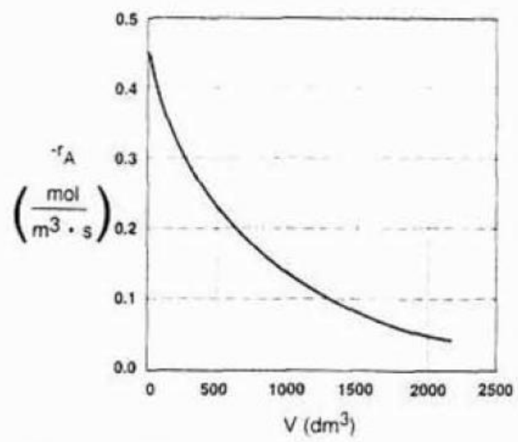


Figure E2-3.2(b) Reaction rate profile.

Q2

$\tau = 5hrs$

$v_0 = 1dm^3/min = 60dm^3/hr$ $C_A = 2.5$ mol/dm^3 $X = 0.8$

For CSTR, $\tau = \dfrac{V}{v_0}$

$V = 300dm^3$

(1)

$$-r_A = \frac{C_{A0}X}{\tau} = \frac{2.5 \times 0.8}{5} mol/dm^3hr$$

$$= 0.4 mol/dm^3hr$$

(2) $V = 300dm^3$

(3) $C_A = C_{A0}(1-X)$

$= 0.5$ mol/dm^3