Problems on CSTR

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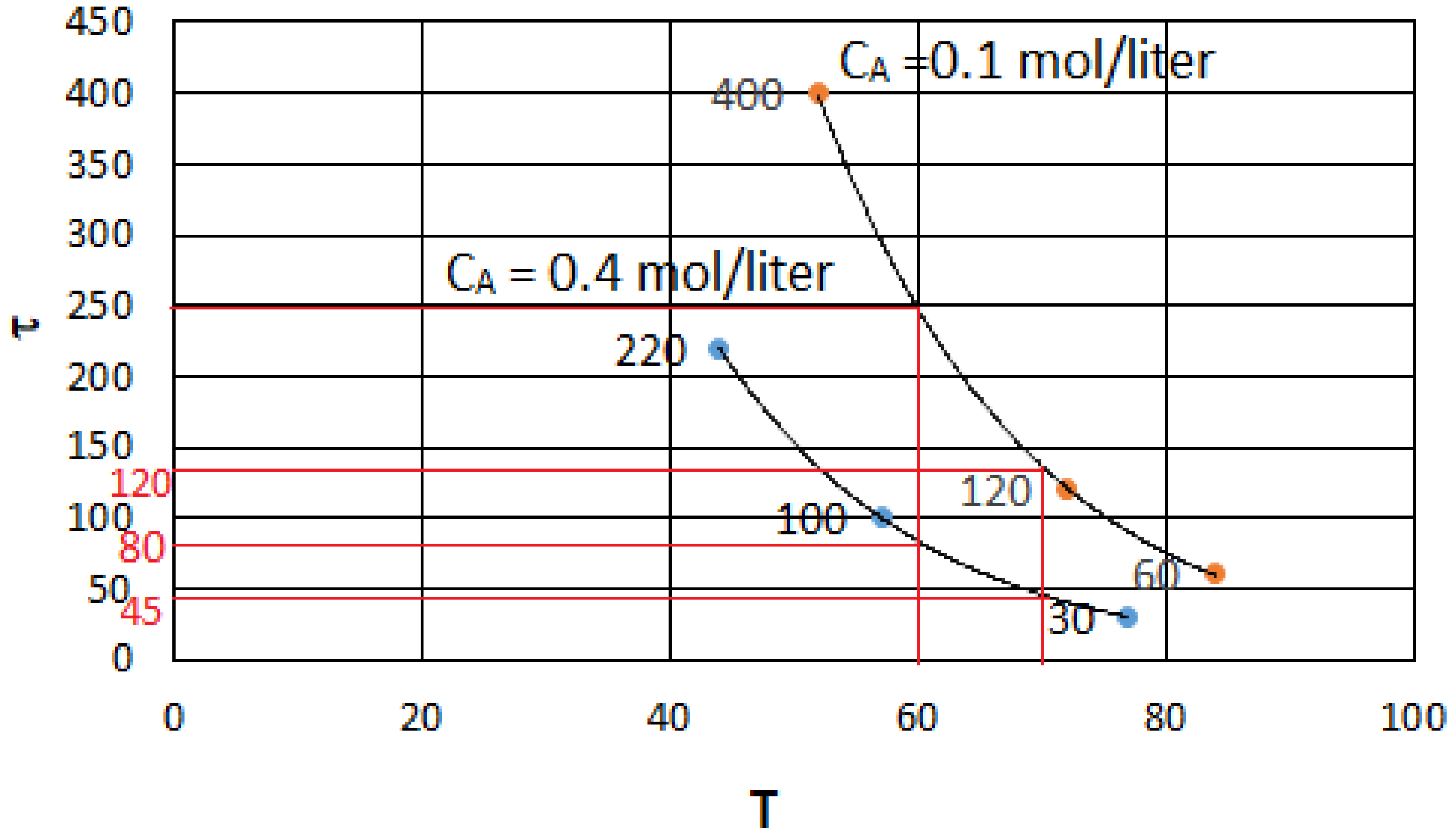
Problem1:

Find the rate equation for the decomposition of liquid A from the results of the kinetic runs conducted in a mixed reactor under steady state conditions.

Concentration of A in Feed, mol/liter	Concentration of A at the exit, mol/liter	Mean residence time of fluid in reactor, sec	Temperature, ^0C
1.0	0.4	220	44
1.0	0.4	100	57
1.0	0.4	30	77
1.0	0.1	400	52
1.0	0.1	120	72
1.0	0.1	60	84

- Solution: For mixed flow reactor
- For constant density system, mean residence time= space time in the reactor,τ
- $\tau = \frac{C_{A0}-C_A}{(-r_A)}$
- $-r_A = \frac{C_{A0}-C_{Af}}{\tau}$
- Plot a graph $\tau \ vs.\ T$ for $C_A = 1.0\ to\ \ C_A = 0.4\ and\ (ii) C_A = 1.0\ to\ \ C_A = 0.1$

Space time versus Temperature Plot



- At $T_1 = 60^0C$, $= 333$ K
- For $C_A = 0.4$ mol/L, $\tau = 80$ s , $C_A = 0.1$ mol/L, $\tau = 250$ s
- $(-r_A)_1 = \frac{C_{A0} - C_{Af}}{\tau} = \frac{1-0.4}{80} = 7.5 \times 10^{-3} mol/(l.s)$
- $ln(-r_A)_1 = -4.89$
- $C_A = 0.1$ mol/L, $\tau = 250$ s
- $(-r_A)_2 = \frac{C_{A0} - C_{Af}}{\tau} = \frac{1-0.1}{250} = 3.6 \times 10^{-3} mol/(l.s)$
- $ln(-r_A)_1 = -5.63$
- Assuming a rate equation of the type
- $-r_A = k\, C_A^n \quad or, \;\; \ln(-r_A) = \ln k + n \ln C_A$

- C_A= 0.1 mol/L, $\ln(-r_A) = \ln k + n \ln C_A$
- $-5.63 = \ln k + n\,(-2.3)$
- C_A= 0.4 mol/L, $-4.89 = \ln k + n\,(-0.92)$
- 0.74= n (1.38)
- n=0.54
- For C_A= 0.4 mol/L,

$$(-r_A)_1 = 7.5 \times \frac{10^{-3} mol}{l.s}$$

- $k = \frac{7.5\times10^{-3}}{0.4^{0.54}} = 0.0123$
- For C_A= 0.1 mol/L, $(-r_A)_2 = 3.6 \times 10^{-3} \times \frac{10^{-3} mol}{l.s}$
- $k = \frac{3.6\times10^{-3}}{0.1^{0.54}} = 0.0123$

- So for two different concentrations k value is constant.
- **Case-2**
- Similarly,
- At T_2 =70^0C, =343 K
- For C_A= 0.4 mol/L, τ= 45 s ,
- $(-r_A)_1 = \frac{C_{A0}-C_{Af}}{\tau} = \frac{1-0.4}{45} = 13.3 \times 10^{-3} mol/(l.s)$
- C_A= 0.1 mol/L, τ= 140 s,
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- $(-r_A)_2 = \frac{C_{A0}-C_{Af}}{\tau} = \frac{1-0.1}{140} = 6.429 \times 10^{-3} mol/(l.s)$
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C_A= 0.1 mol/L, $\ln(-r_A) = \ln k + n \ln C_A \qquad or, \quad -5.05 = \ln k + n\,(-2.3)$

C_A= 0.4 mol/L

$$-4.32 = \ln k + n\,(-0.92)$$

- $-0.73 = n \times (-1.38)$
- Order n=0.53
- At T_1 =70^{0}C, =343 K,
- C_A= 0.4 mol/L
- $(-r_A)_1 = 13.3 \times 10^{-3} mol/(l.s)$
- $k = \frac{13.3\times10^{-3}}{0.4^{0.53}} = \frac{0.0133}{0.615} = 0.02162$
-

- C_A= 0.1 mol/L
- $k = \frac{6.429\times10^{-3}}{0.1^{0.53}} = \frac{0.0064}{0.2951} = 0.02168$
- Average value ok
- At T= 343 K, k=(0.02162+0.02168)/2=0.02165
- At T_1, =333 K, k_1 = 0.0125, and at T_2 = 343, k_2 = 0.02165
- $We\ have\ \ \ lnk = lnk_0 - \frac{E}{RT}$
- $\ln(0.0125) = lnk_0 - \frac{E}{2\times333}\ \ \ or, -4.382 = lnk_0 - \frac{E}{666}$
- $\ln(0.02165) = lnk_0 - \frac{E}{2\times343}\ \ \ or, -3.833 = lnk_0 - \frac{E}{686}$
- $4.382 - 3.833 = \frac{E}{666} - \frac{E}{686} = E(1.501\times10^{-3} - 1.4577\times10^{-3}) = 4.3\times10^{-5}E$

$$E = 12767.4\ cal/mol$$

$$-3.833 = lnk_0 - \frac{12767.4}{686} \quad \Longrightarrow k_0 = 2.619 \times 10^6$$

$$-r_A = k\ C_A^n = 2.619 \times 10^6 e^{-12767/RT} {C_A}^{0.535} \quad Answer$$

Problem-2

- An aqueous feed of A and B(400 lit/min) with C_{A0} =100 mmol/lit and C_{B0} = 200 mmol/lit is to be converted into a product in a mixed flow reactor. The kinetics and stoichiometry of the reaction are given by
- $A + B \rightarrow R, \quad -r_A = 200 C_A C_B \, mol/(lit.\mathrm{min})$
- Estimate the volume of mixed flow reactor required to achieve 99% conversion of A to product.
- Solution:
- $C_A = C_{A0}(1 - X_A) \quad , C_B = C_{B0}(1 - X_B)$
- $C_{A0}X_A = C_{B0}X_B$
- $C_B = C_{B0} - C_{A0}X_A) = C_{A0}(M - X_A) \ where, \ M = C_{B0}/C_{A0}$

$$-r_A = 200 C_A C_B = 200 C_{A0}^2 (1 - X_A)(M - X_A)$$

For mixed flow reactor, the mole balance is

$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} \quad or, \quad V = \frac{C_{A0} X_A}{200 \times C_{A0}^2 (1 - X_A)(M - X_A)}$$

$$C_{A0} = 100 mmol/lit, C_{B0} = 100\ mmol/lit$$

$$C_{A0} = 0.1 mol/lit, C_{B0} = 0.2 mol/lit$$

$$M = \frac{C_{B0}}{C_{A0}} = 2$$

$$X_A = 0.99, \qquad v_0 = 400\ lit/min$$

- $V = \frac{C_{A0} v_0 X_A}{200 \times C_{A0}^2 (1 - X_A)(M - X_A)} = \frac{0.1 \times 400 \times 0.99}{200 \times 0.1^2 \times (1 - 0.99)(2 - 0.99)}$
- $Volume\ of\ mixed\ flow\ reactor,\ \ V = 1960.4\ lit\ \ \ Answer$

Problem-3

Gaseous reactant A decomposes as per the following reaction stoichiometry and kinetics.

$$A \rightarrow 3R \quad -r_A = 0.6\, C_A\, mol/(l.\mathrm{min})$$

Determine the conversion of A in a 50% A and 50% inert feed with v_0 = 180 lit/min ($C_{A0} = 330\, mmol/lit$) to a 1000 liter mixed flow reactor.

Solution: $\epsilon_A \neq 0$

100 mol A + 100 mol reactant = 200 mol of feed

300 mol R + 100 mol Product = Total 400 mol

$$\epsilon_A = \frac{400 - 200}{200} = 1.0$$

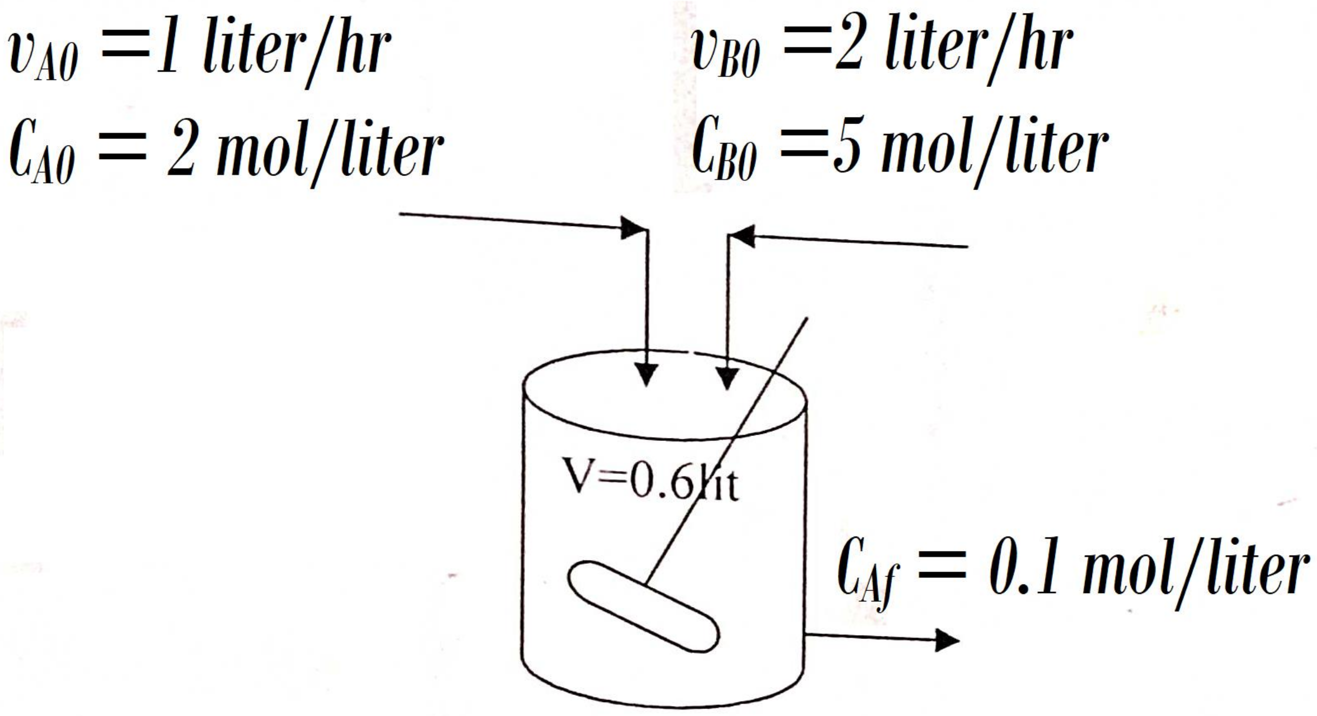
Alternative method: $y_{A0} = 0.5,\ \partial = 3 - 1 = 2,\ \epsilon_A = 2\ \times 0.5 = 1.0$

- $\frac{V}{F_{A0}} = \frac{X_A}{-r_A},\quad or,\quad \tau = \frac{C_{A0}X_A}{-r_A}$
- $-r_A = 0.6\ C_A$
- $C_A = \frac{C_{A0}(1-X_A)}{1+X_A}$
- $\tau = \frac{C_{A0}X_A(1+X_A)}{0.6C_{A0}(1-X_A)}$
- $\tau = \frac{1000}{180} = 3.33 = \frac{X_A(1+X_A)}{0.6(1-X_A)} \Longrightarrow \frac{X_A+X_A^2}{0.6-0.6X_A}$

- $X_A^2 + 4.33X_A - 3.33 = 0$
- $X_A = \frac{-4.33 \pm \sqrt{(4.33)^2 - 4\times1\times(-3.33)}}{2} = 0.67(+ve\ root)$ Answer

Problem 4:

For a second order liquid-phase reaction A + B → P +Q , evaluate the rate constant using the data obtained in a CSTR.



Solution: $v_0 = v_{A0} + v_{B0}$ = 1lit/hr + 2 lit/hr= 3 lit/hr

$F_T = F_{A0} + F_{B0} = C_{A0}\, v_{A0} + C_{B0}\, v_{B0} = 1 \times 2 + 2 \times 5 = 12$ mol/hr

As F_{A0} = 2 mol/hr, F_{B0} = 10 mol/hr.

$C'_{A0} = F_{A0} / v_0 = 2/3 = 0.666$ mol/lit

$C'_{B0} = F_{B0} / v_0 = 10/3 = 3.333$ mol/lit

$$X_A = \frac{0.666 - .1}{0.666} = 0.85$$

$$-r_A = \frac{X_A v_0 C_{A0}}{V} = \frac{0.85 \times 2}{0.6} = 2.833 \text{ mol/lit-hr}$$

$$-r_A = kC'_{A0}(1 - X_A)(C'_{B0} - C'_{A0}X_A) = k(0.0999)(2.767) = k$$

$$k = \frac{2.833}{0.2764} = 10.249\ lit/(mol\ \text{hr}) \text{ Answer}$$