Problems on PFR

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Problem 1. In an isothermal batch reactor the conversion of a liquid reactant A is 70% in 13 min. Find the space time and space velocity necessary to effect this conversion in a plug flow reactor and mixed flow reactor. Consider the first order kinetics.

Solution:

Rate equation : $-r_A = kC_A$

$$-\ln(1 - X_A) = kt$$
$$X_A = 0.70, \qquad for, t = 13\,min$$
$$k = 0.0926\,min^{-1}$$

For mixed reactor,

$$\tau = \frac{C_{A0}X_A}{-r_A} = \frac{C_{A0}X_A}{kC_{A0}(1-X_A)} = \frac{0.70}{0.0926\times(1-0.7)} = 25.2\,min$$

For constant density system and plug-flow reactor

$$t_{batch} = \tau_{plug}$$

- $\frac{\boldsymbol{V}}{\boldsymbol{F_{A0}}} = \int_{\mathbf{0}}^{\boldsymbol{X_{Af}}} \frac{\boldsymbol{dX_A}}{\boldsymbol{-r_A}}$ ***or,*** $\frac{\boldsymbol{\tau}}{\boldsymbol{C_{A0}}} = \int_{\mathbf{0}}^{\boldsymbol{X_{Af}}} \frac{\boldsymbol{dX_A}}{\boldsymbol{-r_A}}$
- $\tau = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{kC_{A0}(1-X_A)} = \int_{\mathbf{0}}^{\boldsymbol{X_{Af}}} \frac{\boldsymbol{dX_A}}{\boldsymbol{k(1-X_A)}}$
- $\tau = \frac{1}{k}[-\ln(1-X_A)]_0^{0.7} = \frac{1}{0.0926}[-\ln(1-0.7)] = 13\,\mathrm{min}\ Answer$

- Problem 2 Assuming a stoichiometry $A \rightarrow R$ for a first order gas phase reaction, the size of a plug flow reactor for 99% conversion of pure A calculated to be 32 liters. In fact, however, the stoichiometry of the reaction $A \rightarrow 3R$. For this corrected stoichiometry, find the required volume of the reactor.
- Solution: Rate equation : $-r_A = kC_A$, ε_A=0,
- $\frac{V}{F_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$
- $\frac{V}{v_0} = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{kC_{A0}(1-X_A)}$
- $\frac{V}{v_0} = \frac{1}{k} ln\left(\frac{1}{1-X_A}\right)$ or, $\frac{32}{v_0} = \frac{1}{k} ln\left(\frac{1}{1-0.99}\right)$
- $\frac{k}{v_0} = 0.144$
- For the corrected stoichiometry $A \rightarrow 3R$
- $\varepsilon_A = \frac{3-1}{1} = 2$

$$\tau = C_{A0} \int_{X_{Ai}}^{X_{Af}} \frac{(1 + \varepsilon_A X_A) dX_A}{k C_{A0} (1 - X_A)}$$

$$V \left(\frac{k}{v_0} \right) = \int_0^{X_A} \frac{dX_A}{1 - X_A} + \varepsilon_A \int_0^{X_A} \frac{X_A dX_A}{1 - X_A}$$

$$V \frac{k}{v_0} = -(1 + \varepsilon_A) \, ln(1 - X_A) - \varepsilon_A X_A$$

$$V \times 0.144 = -(1 + 2) \, ln(1 - 0.99) - 2 \times 0.99$$

$$V = 82.2 \, lit$$

So, the reactor volume with the corrected stoichiometry = 82.2 lit

- Problem 3: The liquid phase decomposition of A is studied in a mixed flow reactor. The results of steady state runs are tabulated below. Find the holding time required (i) in aplug flow reactor as well as (ii) in a mixed flow reactor to obtain 75% conversion of reactant in a feed with C_{A0} = 0.8 mol/lit.

Conc of A in feed stream	**Conc of A in exit stream**	**Holding time (seconds)**
2.0	0.65	300
2.0	0.92	240
2.0	1.00	250
1.0	0.56	110
1.0	0.37	360
0.48	0.42	24
0.48	0.28	200
0.48	0.20	560

- Solution: Liquid phase reaction, $\varepsilon_A = 0$
- $\tau = \frac{C_{A0}X_A}{-r_A} = \frac{C_{A0}-C_A}{-r_A}$
- $\frac{1}{-r_A} = \frac{\tau}{C_{A0}-C_A}$
- Required conversion =0.75 so, required

$C_{Af} = C_{A0}$ (1- X_A)= 0.8(1-.75)=0.2mol/lit

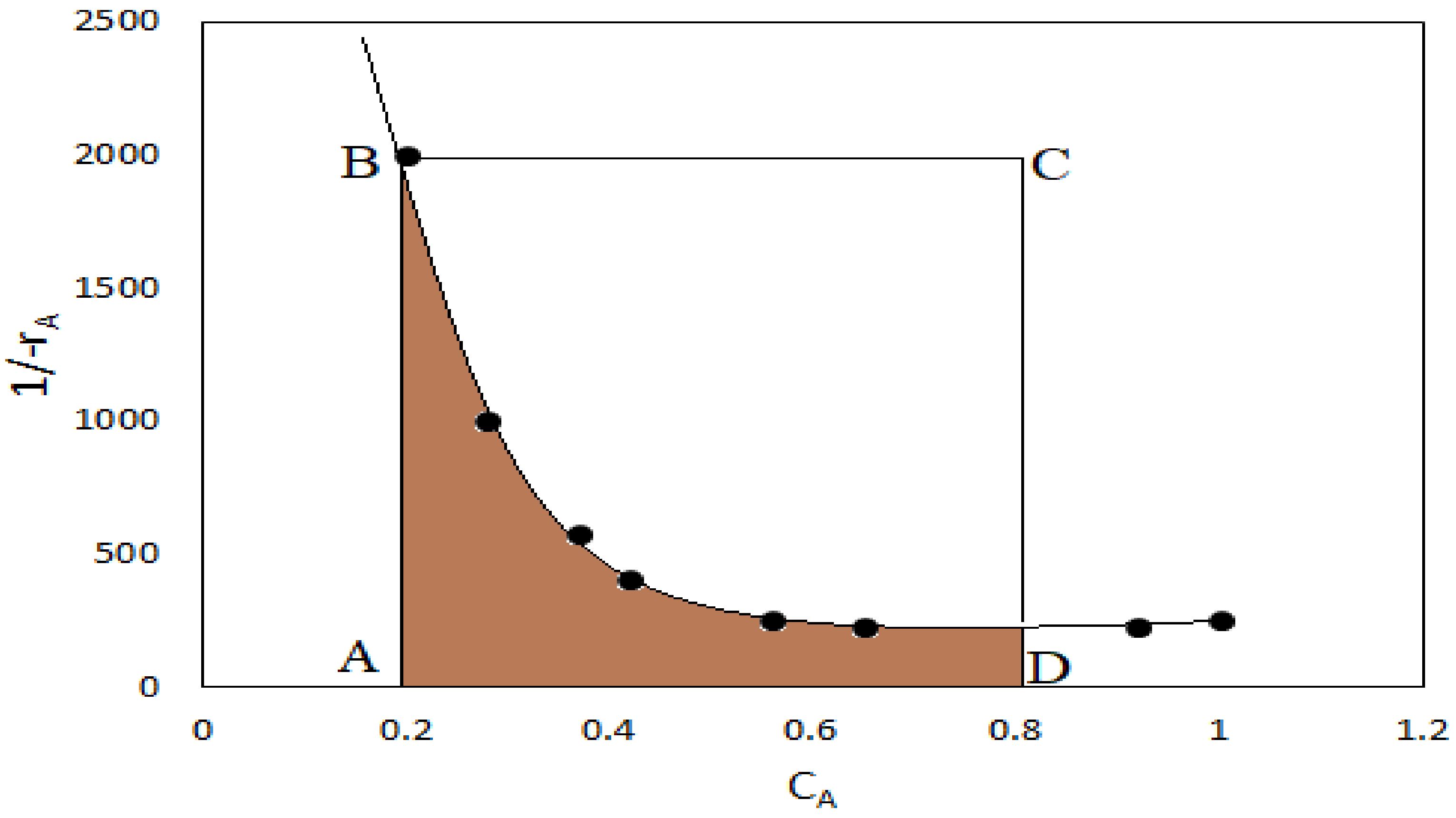
Form the given tabulated data $\frac{1}{-r_A}$ is to calculated for each data point.

For example, for C_{A0} = 2 mol/lit, C_{af} = 0.65, τ =300 seconds

$$\frac{1}{-r_A} = \frac{300}{2-0.65} = 222.22\,\frac{mol}{lit.min}$$

C_A	$1/(-r_A)$
0.65	222.22
0.92	222.22
1.0	250
0.56	250
0.37	571
0.42	400
0.28	1000
0.2	2000

Plot $1/(-r_A)$ as a function of C_A.
τ for mixed flow reactor is the area of rectangle ABCD(area bounded by the rectangle starting from $C_{A0} = 0.8$ and ending at $C_{Af} = 0.2$. τ for PFR is the area under the curve and the x-axis between $C_{A0} = 0.8$ and $C_{Af} = 0.2$



For mixed flow reactor τ_m = area of the rectangle ABCD = 1200 s
and for plug flow reactor = area under the curve (colored section)τ_p = 290 s

Problem 4: A gaseous feed of pure A with C_{A0} =2 mol/lit and F_{A0} =100 mol/min decomposes to give a variety of products in a plug flow reactor. The kinetics and stoichiometry of the reaction are given by

$$A \rightarrow 2.5R\ , -r_A = (10\ min^{-1})C_A$$

Find the conversion that can be obtained in a 22-liter reactor.

Solution: $A \rightarrow 2.5R$ is gaseous reaction so, $\varepsilon_A \neq 0$

$$\varepsilon_A = \frac{2.5 - 1}{1} = 1.5$$

$$\frac{V}{F_{A0}} = \int_{X_{Ai}}^{X_{Af}} \frac{(1 + \varepsilon_A X_A)dX_A}{kC_{A0}(1 - X_A)}$$

$$\frac{V}{F_{A0}} = \frac{1}{kC_{A0}}\left[\int_0^{X_A} \frac{dX_A}{1 - X_A} + \varepsilon_A \int_0^{X_A} \frac{X_A dX_A}{1 - X_A}\right]$$

$$\frac{V}{F_{A0}} = \frac{-(1 + \varepsilon_A)\, ln(1 - X_A) - \ \varepsilon_A X_A}{kC_{A0}}$$

$$\frac{22}{100} = \frac{-(1+1.5)\,ln(1-X_A) - 1.5X_A}{10 \times 2}$$

$4.4 = -2.5\,ln(1-X_A) - 1.5X_A$

By trial and error,

for $X_A = 0.7, RHS = 4.05$
$X_A = 0.750, RHS = 4.591$
$X_A = 0.740, RHS = 4.478$
$X_A = 0.735, RHS = 4.4225$
$X_A = 0.734, RHS = 4.412$
$X_A = 0.733, RHS = 4.4005$

Therefore, $X_A = 0.733, is\ the\ correct\ conversion, i.e$ 73.3 %

Problem -5 : At 600 K the gas-phase reaction

$$C_2H_4 + Br_2 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C_2H_4Br_2$$

has rate constant

$$k_1 = 500 \text{ liter/mol}\cdot\text{hr} \qquad k_2 = 0.032 \text{ hr}^{-1}$$

If a plug flow reactor is to be fed $600\ m^3/hr$ of gas containing 60% Br_2 and 30% C_2H_4 and 10% inerts by volume at 600 K and 1.5 atm compute

(a) the maximum possible fractional conversion of C_2H_4 into $C_2H_4Br_2$

(b) the volume of reaction vessel required to obtain 60% of this maximum conversion.

Solution :

$$\underset{(A)}{C_2H_4} + \underset{(B)}{Br_2} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \underset{(C)}{C_2H_4Br_2}$$

$$-r_{C_2H_4} = k_1 [C_2H_4][Br_2] - k_2 [C_2H_4Br_2]$$

$$K_c = \frac{k_1}{k_2} = \frac{C_C}{C_A C_B} = \frac{(C_{C0} + C_{A0} x_{Ae})(1 + \varepsilon_A x_A)}{C_{A0}(1 - x_{Ae})(C_{B0} - C_{A0} x_{Ae})}$$

$\pi_0 = 1.5$ atm

$$C_{A0} = \frac{1.5 \times 0.3}{0.082 \times 600} = 0.009135 \ \frac{gmol}{lit}$$

$P_{A0} = 1.5 \times 0.3$

$$A + B \rightleftharpoons C$$

$$0.3\,A + 0.6\,B + 0.1\,I \rightleftharpoons 0.3\,C + 0.1\,I + 0.3\,B$$

$$\varepsilon = \frac{0.7 - 1}{1} = -0.3$$

or $\varepsilon = y_{A0}\,\delta$
$= 0.3(-1)$
$= -0.3$

$$C_A = \frac{C_{A0}(1 - x_A)}{1 - 0.3x_A} \qquad C_B = \frac{C_{B0} - C_{A0} x_A}{1 - 0.3\,x_A}$$

$$C_c = \frac{C_{A0} x_A}{1 - 0.3x_A}$$

ε =

$$-r_A = 500 \times .00914 \frac{(1-x_A)}{1-0.3x_A} \times \frac{(.0183 - 0.00914x_A)}{1-0.3x_A}$$

$\boxed{\text{As } C_{B0} = 0.0183}$

$$- .032 \times \frac{0.00914\, x_A}{1-0.3x}$$

$\boxed{C_{A0} = 0.00914}$

$$= \frac{0.04177 \times (1-x_A)(2-x_A)}{(1-0.3x_A)^2} - \frac{292.48 \times 10^{-6}\, x}{1-0.3x_A}$$

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$= C_{A0} \int_0^{x_A} \frac{dx_A}{\frac{0.04177(1-x_A)(2-x_A)}{(1-0.3x_A)^2} - \frac{292.48 \cdot 10^{-6}\, x_A}{(1-.3x_A)}}$$

At equilibrium $x_A = x_{Ae}$

$$0.04177 \frac{(1-x_{Ae})(2-x_{Ae})}{(1-0.3x_{Ae})^2} = 292.48\times10^{-6}\frac{x_{Ae}}{(1-0.3x_{Ae})}$$

$$0.04177 \times (1-x_{Ae})(2-x_{Ae}) = 292.48\times10^{-6}\times x_{Ae}(1-0.3x_{Ae})$$

or $x_{eq} \approx 1.0$ $\therefore$ $x_A = 0.6$

x_A	$f(x)$
0.1	0.0758
0.2	0.068
0.3	0.06
0.4	0.0516
0.5	0.043
0.6	0.0345

on Integration. $\tau = 0.00914 \times 10.7$

$= 0.0978$

Volume of ~~reaction~~ $= 600 \times 0.0978$

$= 58.678 \ m^3$ Ans