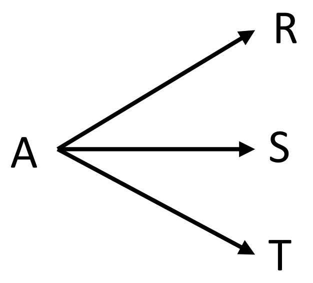
Problems on Multiple Reactions

J. K. Basu

1. Liquid reactant A decomposes as per the following parallel reactions:



With $r_R = 1$, $r_S = 2\,C_A$, $r_T = C^2_A$, $C_{A0} = 2$

Determine the maximum concentration of the desired product (C_S) that can be obtained.

(a) in a mixed flow reactor
(b) in a plug flow reactor
(c) in any reactor of your choice if unreacted A can be separated from the product stream and returned to the feed.

As S is the desired product, fractional yield in terms of S can be written as

$$\varphi(S/A) = \frac{dC_S}{dC_R + dC_S + dC_T} = \frac{2C_A}{1 + 2C_A + C_A^2} = \frac{2C_A}{(1 + C_A)^2}$$

$$\frac{d\varphi}{dC_A} = \frac{d}{dC_A}\left[\frac{2C_A}{(1 + C_A)^2}\right] = 0$$

$$\frac{(1 + C_A)^2 - C_A(2 + 2C_A)}{(1 + C_A)^4} = 0$$

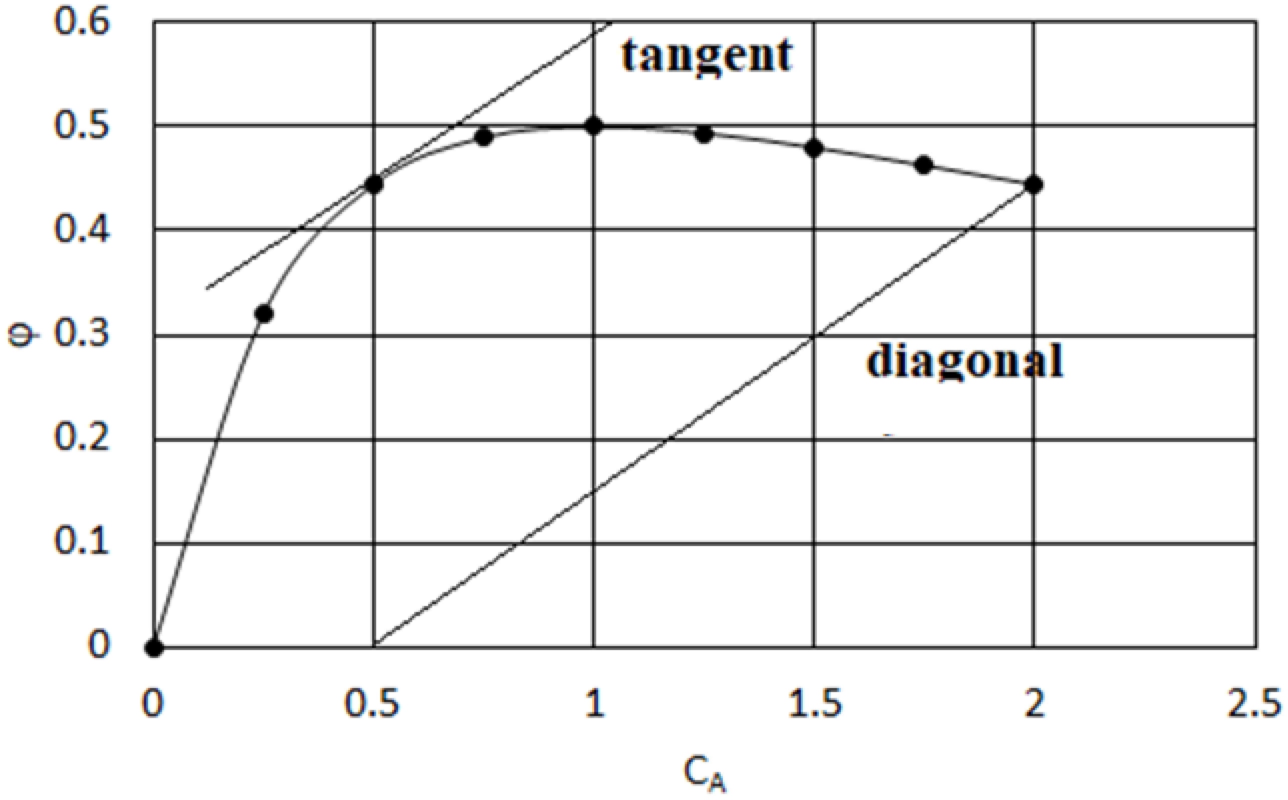
$$(1 + C_A) - 2C_A = 0$$
$$C_A = 1 \; or \; C_{Af} = 1$$

$$\varphi(S/A) = \frac{2C_A}{(1 + C_A)^2} = \frac{2}{(1 + 1)^2} = 0.5\,, the\ maximum\ \varphi(S/A)$$

Graphical method

$$\varphi(S/A) = \frac{2C_A}{(1+C_A)^2},$$

At various values of C_A, calculate $\varphi(S/A)$ and plot keeping φ in y-axis and C_A in x-axis.



Mixed flow reactor: The maximum S will form when area under the curve φ vs C_A is the largest

- When diagonal of the rectangle = slop of the tangent as shown in the figure.
- For C_{Af} =0.5, it is occurred. C_{Sf} will be obtained finding the area of the rectangle between C_{A0} = 2 and C_{af} =0.5, i.e. area= 0.44×1.5 = 0.66

so, C_{Sf} = 0.66mol/lit.

Analytical Method:

$$C_{Sf} = \varphi \times (-\Delta C_A) = \frac{2C_A}{(1+C_A)^2}(C_{A0} - C_A)$$

The optimum value of C_{Sf} is obtained by

$$\frac{dC_{Sf}}{dC_A} = 0$$

$$\frac{d}{dC_A}\left[\frac{2C_A}{(1+C_A)^2}(C_{A0} - C_A)\right] = 0$$

- $\frac{d}{dC_A}\left[\frac{2C_A}{(1+C_A)^2}(2-C_A)\right] = 0$

$2\times\frac{(1+C_A)^2(2-2C_A)-(2C_A-C_A^2)(2+2C_A)}{(1+C_A)^4} = 0$

- $4\times\frac{(1+C_A)^2(1-C_A)-(2C_A-C_A^2)(1+C_A)}{(1+C_A)^4} = 0$
- $1-C_A^2-2C_A+C_A^2 = 0$
- $C_A = 0.5 mol/lit$
- $C_S = \frac{2C_A}{(1+C_A)^2}(2-C_A) = \frac{2\times 0.5}{(1.5)^2}(2-0.5) = 0.666 mol/lit$

Plug flow reactor

The formation of S is maximum when area under the curve is maximum. This occurs at 100% conversion i.e C_{Af} =0.

C_{Sf} =0.8625(by graphical method)

Analytical method

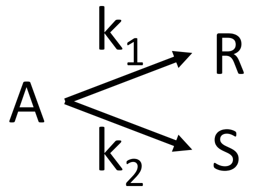
$$C_{Sf} = -\int_0^2 \frac{2C_A}{(1+C_A)^2} dC_A$$

Assume, x=1 + C_A

$$2\int_1^3 \frac{(x-1)}{(x)^2} dx = 2\left[(lnx)_1^3 - \left(\frac{-1}{x}\right)_1^3\right] = 0.864\text{mol/lit}$$

In PFR the formation of S is largest.

2. Liquid reactant A decomposes as per the following reaction scheme:



Rates are : $r_R = k_1 C_A^2$, $r_S = k_2 C_A$, $k_1 = 0.4 m^3/(mol.min)$ $k_2 = 2\, min^{-1}$

An aqueous feed containing A with $C_{A0} = 40\, mol/m^3$ is used.

A mixture of A, R and S leaves the reactor. Find the operating conditions.

X_A ,τ and C_R which maximizes C_R in a mixed flow reactor.

Solution:

$$\varphi(R/A) = \frac{dC_R}{dC_R + dC_S} = \frac{k_1 C_A^2}{k_1 C_A^2 + k_2 C_A} = \frac{0.4 C_A^2}{0.4 C_A^2 + 2 C_A} = \frac{1}{1 + \frac{5}{C_A}}$$

$$C_{Rf} = \varphi(R/A) \times (-\Delta C_A) = \frac{1}{1 + \frac{5}{C_A}} (C_{A0} - C_A)$$

$$\frac{dC_{Rf}}{dC_A} = 0$$

$$\frac{d}{dC_A}\left[\frac{C_{A0}}{1+\frac{5}{C_A}}(C_{A0} - C_A)\right] = 0$$

$$\frac{-C_{A0}\frac{-5}{C_A^2} - \left[1 + \frac{5}{C_A} - C_A\left(\frac{-5}{C_A^2}\right)\right]}{\left(1+\frac{5}{C_A}\right)^2} = 0$$

$$\frac{5C_{A0}}{C_A^2} - 1 - \frac{5}{C_A} - \frac{5}{C_A} = 0$$

$C_A^2 + 10C_A - 200 = 0 \; for \; C_{A0}$ =40 C_A=10 mol/m^3 +ve root

Maximum R is formed for C_{Af} =10 mol/m^3

$$C_{Rf} = \frac{1}{1+\frac{5}{C_A}}(C_{A0} - C_A) = \frac{1}{1+\frac{5}{10}}(40-10) = 20 mol/m^3$$

$$X_A = \frac{40-10}{40} = 0.75$$

$$\tau = \frac{C_{A0}X_A}{-r_A} = \frac{C_{A0}X_A}{k_1 C_A^2 + k_2 C_A} = \frac{C_{A0}X_A}{k_1 C_{A0}^2(1-X_A)^2 + k_2 C_{A0}(1-X_A)}$$
$$= \frac{0.75}{0.4 \times 40 \times (1-0.75)^2 + 2 \times (1-0.75)}$$

$$\tau = 0.5\, min$$

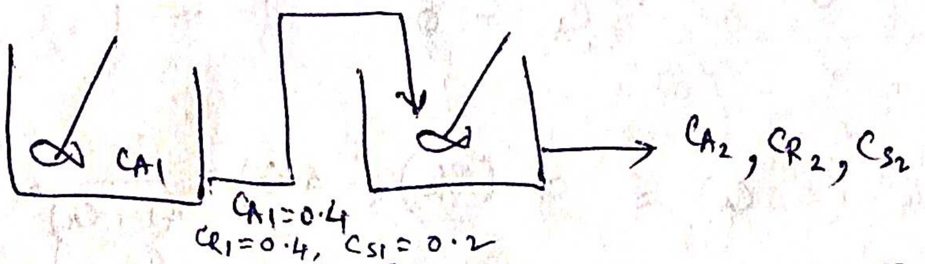
Prob -3 Substance A in the liquid phase produces R and S by the following reactions:

$$A \xrightarrow{k_1} R \qquad r_R = k_1 C_A^2$$

$$A \xrightarrow{k_2} S \qquad r_S = k_2 C_A$$

The feed containing $C_{A0} = 1.0$ moles/liter, $C_{R0} = 0$ and $C_{S0} = 0$ enter two CSTR in series ($\tau_1 = 2.5$ min, $\tau_2 = 10$ min). $C_{A1} = 0.4$ moles/liter, $C_{R1} = 0.4$ moles, $C_{S1} = 0.2$ find the composition leaving second reactor

Solution:



$$-r_A = k_1 C_A^2 + k_2 C_A \qquad \tau_1 = \frac{C_{A0} - C_{A1}}{(-r_A)_1}$$

$$\tau_1 = \frac{C_{A0} - C_{A1}}{(-r_A)_1}$$

$$2.5 = \frac{1 - 0.4}{k_1 (0.4)^2 + k_2 (0.4)}$$

or $$0.4 k_1 + k_2 = 0.6$$

$$\tau_1 = \frac{C_{R1} - C_{R0}}{r_R} \Rightarrow 2.5 = \frac{0.4}{k_1 (0.4)^2}$$

$$k_1 = 1$$

$\therefore$ $$k_2 = 0.6 - 0.4 = 0.2$$

$$\tau_2 = \frac{C_{A1} - C_{A2}}{(-r_A)_2}$$

or $$10 = \frac{0.4 - C_{A2}}{k_1 C_{A2}^2 + k_2 C_{A2}}$$

$$= \frac{0.4 - C_{A2}}{C_{A2}^2 + 0.2 C_{A2}}$$

$$10 C_{A2}^2 + 2 C_{A2} - 0.4 + C_{A2} = 0$$

or $$10 C_{A2}^2 + 3 C_{A2} - 0.4 = 0$$

$$C_{A2} = \frac{-3 \pm \sqrt{9 + 16}}{20}$$

$$= \frac{-3 \pm 5}{20} \qquad C_{A2} = 0.1, \cancel{-0.4}$$

$$\tau_2 = \frac{C_{R_2} - C_{R_1}}{(r_R)_m}$$

$$10 = \frac{C_{R_2} - 0.4}{(0.1)^2} \quad C_{R_2} = 0.5$$

$$\tau_2 = \frac{C_{S_2} - C_{S_1}}{(r_S)_2} \; ; \quad 10 = \frac{C_{S_2} - 0.2}{(0.2)(0.1)} \qquad C_{S_2} = 0.4$$

$$C_{A_2} = 0.1 \, , \quad C_{R_2} = 0.5 \, , \quad C_{S_2} = 0.4$$

Prob-4 We have a mixture containing 90 mole % A (45 mol/liter) and 10 mole % impurity B (5 mol/liter). To be satisfactory quality the mole ratio of A to B in the mixture must be 100 to 1 or higher. D reacts with both A and B as follows:

$$A + D \rightarrow R, \qquad -r_A = 21\, C_A C_D$$

$$B + D \rightarrow S, \qquad -r_B = 147\, C_B C_D$$

Assuming that the reactions go to completion, how much D need be added to a batch of mixture to bring about the desired quality?

Solution: $\dfrac{C_{A0}}{C_{B0}} = 9, \qquad \dfrac{C_A}{C_B} = 100$

$$\frac{r_B}{r_A} = \frac{147\, C_B C_D}{21\, C_A C_D} = \frac{7\, C_B}{C_A}$$

$$\frac{dC_B}{dC_A} = 7\, C_B / C_A \quad \text{or} \quad \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{C_A} = \frac{1}{7}\int_{C_{B0}}^{C_{Bf}} \frac{dC_B}{C_B}$$

$$\ln \frac{C_{Af}}{C_{A0}} = \frac{1}{7} \ln \frac{C_{Bf}}{C_{B0}}$$

$$\frac{C_{Af}}{C_{A0}} = \left(\frac{C_{Bf}}{C_{B0}}\right)^{1/7} \qquad \frac{100\, C_{Bf}}{C_{A0}} = \frac{(C_{Bf})^{1/7}}{(C_{B0})^{1/7}}$$

$$C_{Bf}^{\,6/7} = \frac{C_{A0}}{100} \times \frac{1}{C_{B0}^{\,1/7}} = \frac{45}{100} \times \frac{1}{5^{1/7}} = 0.358$$

$$C_{Bf} = (0.358)^{7/6} = 0.301 \text{ mol/L}$$

$$C_{Af} = 100 \times 0.301 = 30.1 \text{ mol/L}$$

'D' consumed per liter = (A consumed by 1st reaction) + (B consumed in 2nd reaction)

$$= (45 - 30.1) + (5 - 0.301)$$

$$= 19.6 \text{ moles}$$

19.6 moles/liter of D should be added in the batch.

Prob - 5 A and B react with each other as follows:

$$2A \rightarrow R \qquad r_R = K_1 C_A^2$$

$$A + B \rightarrow S \qquad r_S = K_2 C_A C_B \quad \text{(desired product is S)}$$

$$2B \rightarrow T, \qquad r_T = K_3 C_B^2$$

Find what ratio of A to B should be maintained in a mixed flow reactor to maximize the fractional yield of S, the desired product

Solution: Let $z = \frac{C_A}{C_B}$.

$$\varphi\left(\frac{S}{R+S+T}\right) = \frac{K_2 C_A C_B}{K_1 C_A^2 + K_2 C_A C_B + K_3 C_B^2} = \frac{K_2}{K_1 \frac{C_A}{C_B} + K_2 + K_3 \frac{C_B}{C_A}}$$

$$\phi\left(\frac{S}{R+S+T}\right) = \frac{K_2 \frac{C_A}{C_B}}{K_1\left(\frac{C_A}{C_B}\right)^2 + K_2 \frac{C_A}{C_B} + K_3} = \frac{K_2 Z}{K_1 Z^2 + K_2 Z + K_3}$$

$$\frac{d\phi}{d\left(\frac{C_A}{C_B}\right)} = \frac{d\phi}{dZ} = 0$$

$$\left[K_1 Z^2 + K_2 Z + K_3\right] K_2 - K_2 Z\left[2K_1 Z + K_2\right] = 0$$

$$K_1 K_2 Z^2 + \cancel{K_2^2 Z} + K_2 K_3 - 2 K_1 K_2 Z^2 - \cancel{K_2^2 Z} = 0$$

$$K_1 K_2 Z^2 = K_2 K_3$$

$$Z^2 = \frac{K_2 K_3}{K_1 K_2} = \frac{K_3}{K_1} \qquad \frac{C_A}{C_B} = \sqrt{\frac{K_3}{K_1}}$$

So the required ratio is $\frac{C_A}{C_B}$ should be $\sqrt{\frac{K_3}{K_1}}$

Prob - 6 Equimolar quantities of A, B and D are fed continuously to a mixed flow reactor where they combine by the elementary reactions

$$\left.\begin{aligned} A + D &\xrightarrow{k_1} R \\ B + D &\xrightarrow{k_2} S \end{aligned}\right\} \quad \text{With } \frac{k_2}{k_1} = 0.2$$

(a) If 50 % of the incoming A is consumed find what fraction of the products formed is R

(b) If 50% of the incoming D is consumed find what fraction of the products formed is R

Solution:

(a) $X_A = 0.5$ $\qquad -r_R = k_1 C_A C_D$

$r_S = k_2 C_B C_D$

$$\varphi\frac{R}{S} = \frac{k_1 C_A C_D}{k_1 C_A C_D + k_2 C_B C_D}$$

$$C_{A0} = C_{B0} = C_{D0} = C_0$$

$$\frac{dC_R}{dt} = k_1 C_A C_D \qquad \frac{dC_S}{dt} = k_2 C_A C_D$$

$$\varphi\left(\frac{R}{S}\right) = \frac{C_A}{C_A + \left(\frac{k_2}{k_1}\right) C_B}$$

For mixed reactor

$$\frac{V}{F_{A0}} = \frac{\Delta X_A}{-r_A}$$

$$\frac{\Delta X_A}{-r_A} = \frac{\Delta X_B}{-r_B}$$

$$\frac{x_A}{k_1 C_A C_D} = \frac{x_B}{k_2 C_B C_D}$$

$$x_B = \frac{k_2}{k_1} \frac{C_B}{C_A} x_A = (0.2)\left(\frac{C_B}{0.5\, C_{A0}}\right) 0.5 = 0.2 \frac{C_B}{C_{A0}} = 0.2 \frac{C_B}{C_0}$$

also, $x_B = \frac{C_{B0} - C_B}{C_{B0}} = 1 - \frac{C_B}{C_{B0}} = 1 - \frac{C_B}{C_0}$

$$1 - \frac{C_B}{C_0} = 0.2 \frac{C_B}{C_0} \quad \text{or}, \quad 1.2 \frac{C_B}{C_0} = 1 \quad \text{or} \quad C_B = \frac{1}{1.2} C_0$$

$$\phi\left(\frac{R}{S}\right) = \frac{0.5\, C_0}{0.5\, C_0 + 0.2\left(\frac{1}{1.2}\right) C_0} = 0.75$$

Prob - 7

$A \rightarrow R \qquad r_R = 1$

$A \rightarrow S$ desired $\qquad r_S = 2C_A$

$A \rightarrow T \qquad r_T = C_A^2 \qquad C_{A0} = 2$

S is the desired product.

Find the maximum C_{Sf} can be obtained in PFR and mixed flow reactor.

Solution: $\phi(S/A) = \dfrac{r_S}{r_S + r_R + r_T} = \dfrac{dC_S}{dC_S + dC_R + dC_T} = \dfrac{2C_A}{1 + 2C_A + C_A^2}$

$$= \frac{2C_A}{(1+C_A)^2}$$

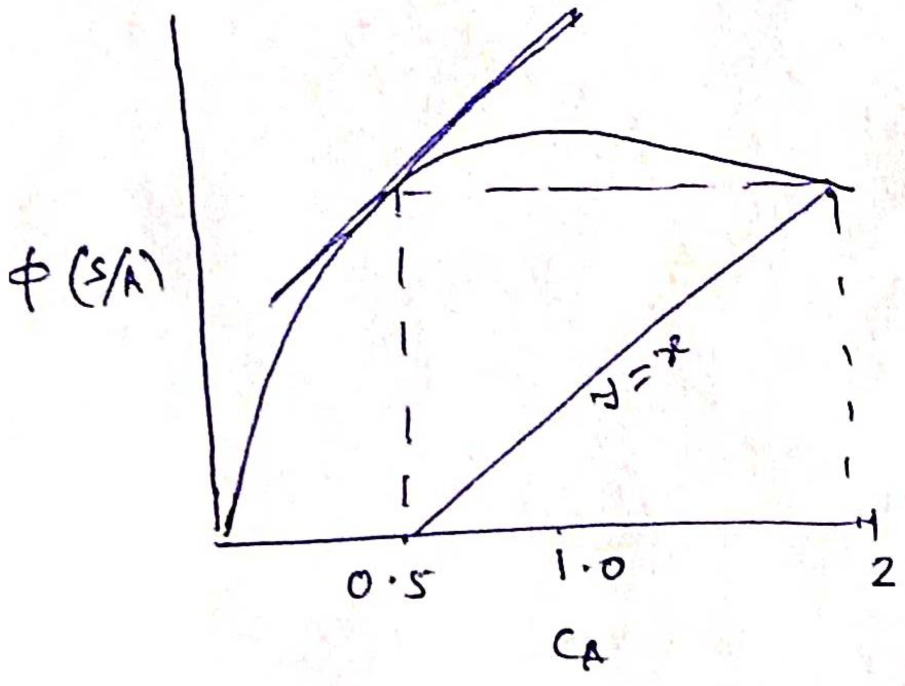
$$\frac{d\phi}{dC_A} = 0 \qquad 2\left[\frac{(1+C_A)^2 \times 1 - C_A(2+2C_A)}{(1+C_A)^4}\right] = 0$$

$$\frac{(1+C_A) - 2C_A}{(1+C_A)^3} = 0 \qquad 1 + C_A - 2C_A = 0 \qquad \begin{array}{l} C_A = 1.0 \\ C_{Af} = 1.0 \end{array}$$

$$\phi_{max} = \frac{2 \times 1}{(1+1)^2} = 0.5$$

for different C_A plot ϕ

C_A	0	0.25	0.5	.75	1	1.25	1.5	1.75	2
$\phi\ (S/A)$	0	0.32	0.44	0.489	.5	0.49	0.48	0.46	0.44



Maximum S is formed when the φ vs C_A curve has the largest area under that curve.

A tangent to the curve will be equal to the diagonal

$C_{Af} = 0.5$ $\quad C_{A0} = 2$

Area $= 26.4\ cm^2$

C_{Sf} = Area × Scale x-axis × Scale y-axis

$= 26.4 \times 0.25 \times 0.1$

$= 0.66$

or $0.44 \times 1.5 = 0.66$

Prob-8 Reactant A in a liquid produces R and S by two parallel

A feed with $C_{A0} = 1$, $C_{R0} = 0$ and $C_{S0} = 0$ enters in two mixed reactors in series ($\tau_1 = 2$ min; $\tau_2 = 4$ min). The composition in the first reactor is $C_{A1} = 0.4$, $C_{R1} = 0.4$ and $C_{S1} = 0.2$, find the composition leaving the second reactor

$$A \nearrow R \quad A \searrow S$$

Solution

$A \rightarrow R$ first-order

$A \rightarrow S$ first-order

$$-r_A = K_1 C_A + K_2 C_A = (K_1 + K_2) C_A$$

$$r_R = K_1 C_A \qquad r_S = K_2 C_A$$

$$\frac{r_R}{r_S} = \frac{dC_R}{dC_S} = \frac{K_1}{K_2}$$

$$\frac{C_R - C_{R0}}{C_S - C_{S0}} = \frac{K_1}{K_2} \qquad C_{R0} = C_{S0} = 0$$

$$\frac{C_R}{C_S} = \frac{0.4}{0.2} = \frac{K_1}{K_2} \qquad \text{As } C_{R_1} = 0.4,\ C_{S_1} = 0.2$$

from first reactor

$$K_1 = 2K_2$$

$$-r_A = (K_1 + K_2)\,C_A = 3K_2\,C_A$$

<u>For mixed reactor</u>

1st- reactor

$$\tau_1 = \frac{C_{A0} - C_{A_1}}{(K_1 + K_2)\,C_{A_1}} = \frac{1 - 0.4}{3K_2\,0.4}$$

$$2 = \frac{0.6}{1.2\,K_2} \Rightarrow K_2 = \frac{0.6}{2.4} = 0.25$$

$$K_1 = 2 \times 0.25 = 0.5 \qquad K_1 + K_2 = 0.75$$

Second reactor

$$\tau_2 = \frac{C_{A1} - C_{A2}}{(-r_A)_2} = \frac{C_{A1} - C_{A2}}{0.75\, C_{A2}}$$

$$4 = \frac{0.4 - C_{A2}}{0.75\, C_{A2}}$$

$$3\, C_{A2} = 0.4 - C_{A2}$$

$$4\, C_{A2} = 0.4 \qquad C_{A2} = 0.1$$

R- balance in 2nd- reactor

$$\tau_2 = \frac{C_{R2} - C_{R1}}{K_1\, C_{A2} \longrightarrow r_R}$$

$$4 = \frac{C_{R2} - 0.4}{0.5\, C_{A2}}$$

$$2\, C_{A2} = C_{R2} - 0.4$$

As $C_{A2} = 0.1$

$$0.2 = C_{R2} - 0.4$$

$$C_{R2} = 0.2 + 0.4 = 0.6$$

S- balance in 2nd-reactor

$$\tau_2 = \frac{C_{S_2} - C_{S_1}}{(r_S)_2} = \frac{C_{S_2} - C_{S_1}}{K_2 C_{A_2}}$$

$$K_2 C_{A_2} \tau_2 = C_{S_2} - C_{S_1}$$

$$C_{S_2} = (K_2 C_{A_2} \tau_2) + C_{S_1}$$

$$= (0.25)(0.1)(4) + 0.2$$

$$= 0.1 + 0.2 = 0.3$$

$$\left.\begin{aligned} C_{A_2} &= 0.1 \\ C_{R_2} &= 0.6 \\ C_{S_2} &= 0.3 \end{aligned}\right\} \text{Ans}$$

Prob-9 Consider the parallel decomposition of A

$$A \begin{cases} \nearrow R \\ \rightarrow S \\ \searrow T \end{cases}$$

With $r_R = 1$, $r_S = 2\,C_A$, $r_T = C_A^2$,

Determine the maximum concentration of the desired product that can be obtained

(i)in a mixed flow reactor and (ii) in a plug flow reactor

(a) R is the desired product with $C_{A0} = 2$

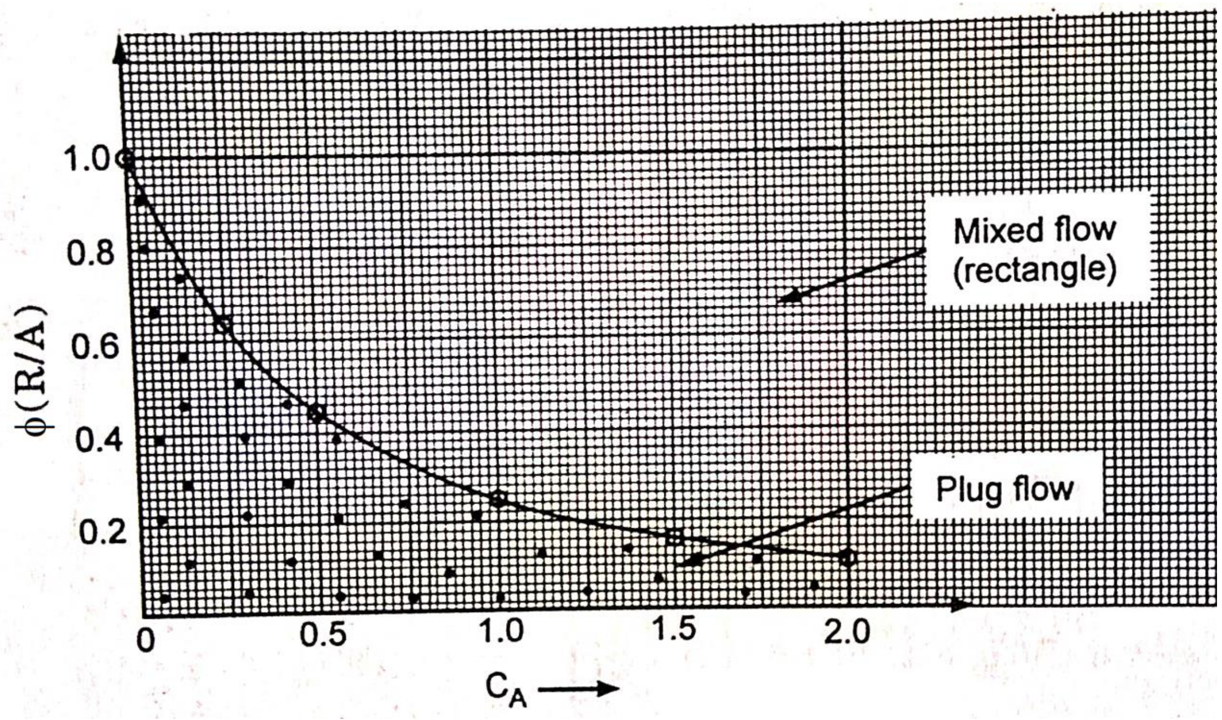
(b) S is the desired product with $C_{A0} = 4$

Solution: R is the desired product with $C_{A0} = 2$

$$\varphi(R/A) = \frac{dC_R}{dC_R + dC_S + dC_T} = \frac{1}{1 + 2C_A + C_A^2} = \frac{1}{(1 + C_A)^2}$$

Take C_A = 0, 0.25 0.5, 1……up to 2, calculate $\varphi(R/A)$

C_A	0	0.25	0.5	1	1.5	2
$\varphi(R/A)$	1	0.64	0.44	0.25	0.16	0.11



For PFR, C_{Af} =0, area is maximum,
C_{Rf} = 0.6625(from area)
For Mixed flow reactor, for C_{Af} =0,
Area of rectangle= 2
C_{Rf} =2

S is the desired product with C_{A0} =4

$$\varphi(S/A) = \frac{dC_S}{dC_R + dC_S + dC_T} = \frac{2C_A}{1 + 2C_A + C_A^2} = \frac{2C_A}{(1 + C_A)^2}$$

$$C_{Sf} = \varphi \times (-\Delta C_A) = \frac{2C_A}{(1 + C_A)^2}(C_{A0} - C_A)$$

$$\frac{dC_{Sf}}{dC_A} = 0$$

$$\frac{d}{dC_A}\left[\frac{2C_A}{(1 + C_A)^2}(4 - C_A)\right] = 0$$

$$\frac{d}{dC_A}\left[\frac{1}{(1 + C_A)^2}(4C_A - C_A^2)\right] = 0$$

$$\frac{(1 + C_A)^2(4 - 2C_A) - (4C_A - C_A^2)(2 + 2C_A)}{(1 + C_A)^4} = 0$$

$$4-2C_A+4C_A-2C_A^2-8C_A+2C_A^2=0$$

$$4-6C_A=0$$

$$C_A=\frac{4}{6}=0.67$$

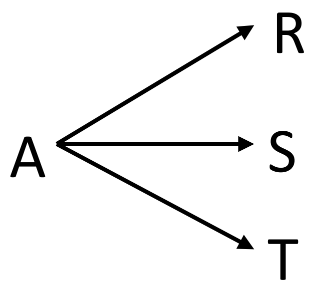
$$C_{Sf}=\varphi\times(-\Delta C_A)=\frac{2\times 0.67}{(1+0.67)^2}(4-0.67)=1.6$$

For plug flow reactor

$$C_{Sf}=-\int_0^4\frac{2C_A}{(1+C_A)^2}dC_A$$

$$2\int_1^5\frac{(x-1)}{(x)^2}dx=2\left[(lnx)_1^5-\left(\frac{-1}{x}\right)_1^3\right]=1.62\text{mol/lit}$$

Prob-10 Consider the parallel decomposition of A of Prob-9



With $r_R = 1$, $r_S = 2\,C_A$, $r_T = C^2{}_A$ with $C_{A0} = 4$

Determine the arrangement of reactors which would produce most S in a flow system where recycle of unreacted feed is not possible. Determine $C_{S,Total}$.

Solution:

$$\varphi(S/A) = \frac{dC_S}{dC_R + dC_S + dC_T} = \frac{2C_A}{1 + 2C_A + C_A^2}$$

$$\varphi(S/A) = \frac{dC_S}{dC_R + dC_S + dC_T} = \frac{2C_A}{1 + 2C_A + C_A^2}$$

$$= \frac{2C_A}{(1 + C_A)^2}$$

$$\frac{d\varphi}{dC_A} = \frac{d}{dC_A}\left[\frac{2C_A}{(1 + C_A)^2}\right] = 0$$

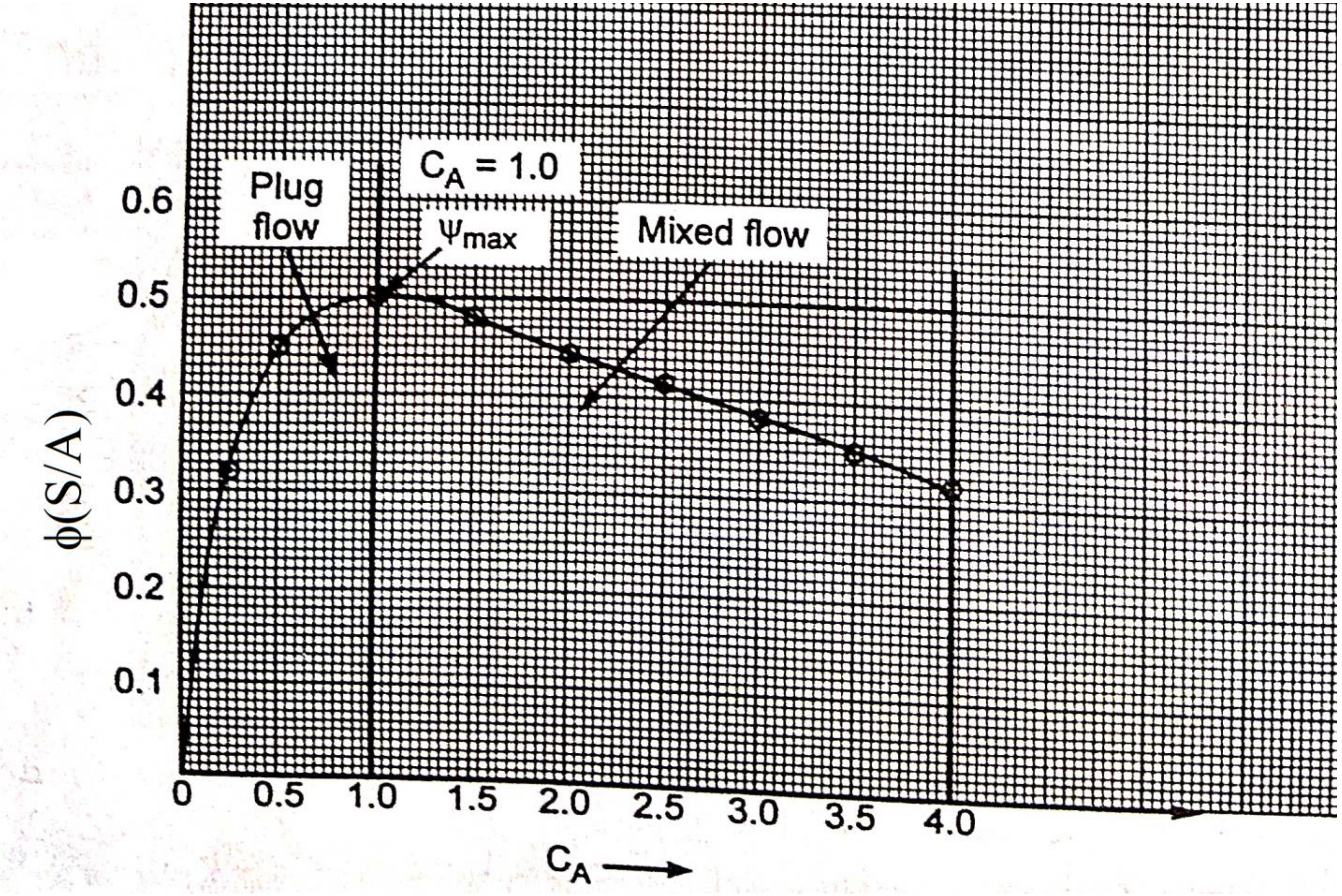
$$\frac{(1 + C_A)^2 - C_A(2 + 2C_A)}{(1 + C_A)^4} = 0$$

$$(1 + C_A) - 2C_A = 0$$

$$C_A = 1 \; or \; C_{Af} = 1$$

$$\varphi(S/A) = \frac{2C_A}{(1 + C_A)^2} = \frac{2}{(1 + 1)^2}$$

$$= 0.5\,, the\ maximum\ \varphi(S/A)$$



If we operate mixed flow reactor from C_{A0} = 4 to C_A = 1.0
(for highest fractional yield of S and followed by a plug flow reactor
Converting from C_{A0} = 1 to C_A = 0.0

For mixed flow reactor $C_S = \varphi \times (-\Delta C_A) = 0.5(4-1) = 1.5$

For plug flow reactor integrate from 0 to 1

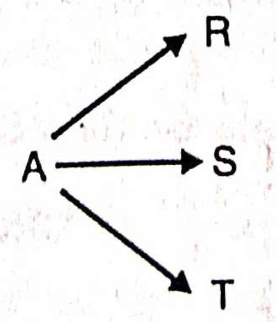
$$C_{Sf} = -\int_0^1 \frac{2C_A}{(1+C_A)^2} dC_A$$

$$2\int_1^3 \frac{(x-1)}{(x)^2} dx = 2\left[(lnx)_1^2 - \left(\frac{-1}{x}\right)_1^2\right] = 0.386$$

$C_{S,\ Total} = 1.5 + 0.386 = 1.886$

Mixed reactor followed by plug flow reactor is the best arrangement.

Prob - 11: Consider the parallel decomposition of A as per the following scheme :



with $r_R = 1.0$, $r_S = 2\,C_A$ and $r_T = C_A^2$.

Determine the maximum concentration of desired product that can be obtained in (i) a plug flow reactor and (ii) in a mixed flow reactor. For : T is the desired product and $C_{A_0} = 5$.

Solution : $A \to R$, $r_R = 1.0$

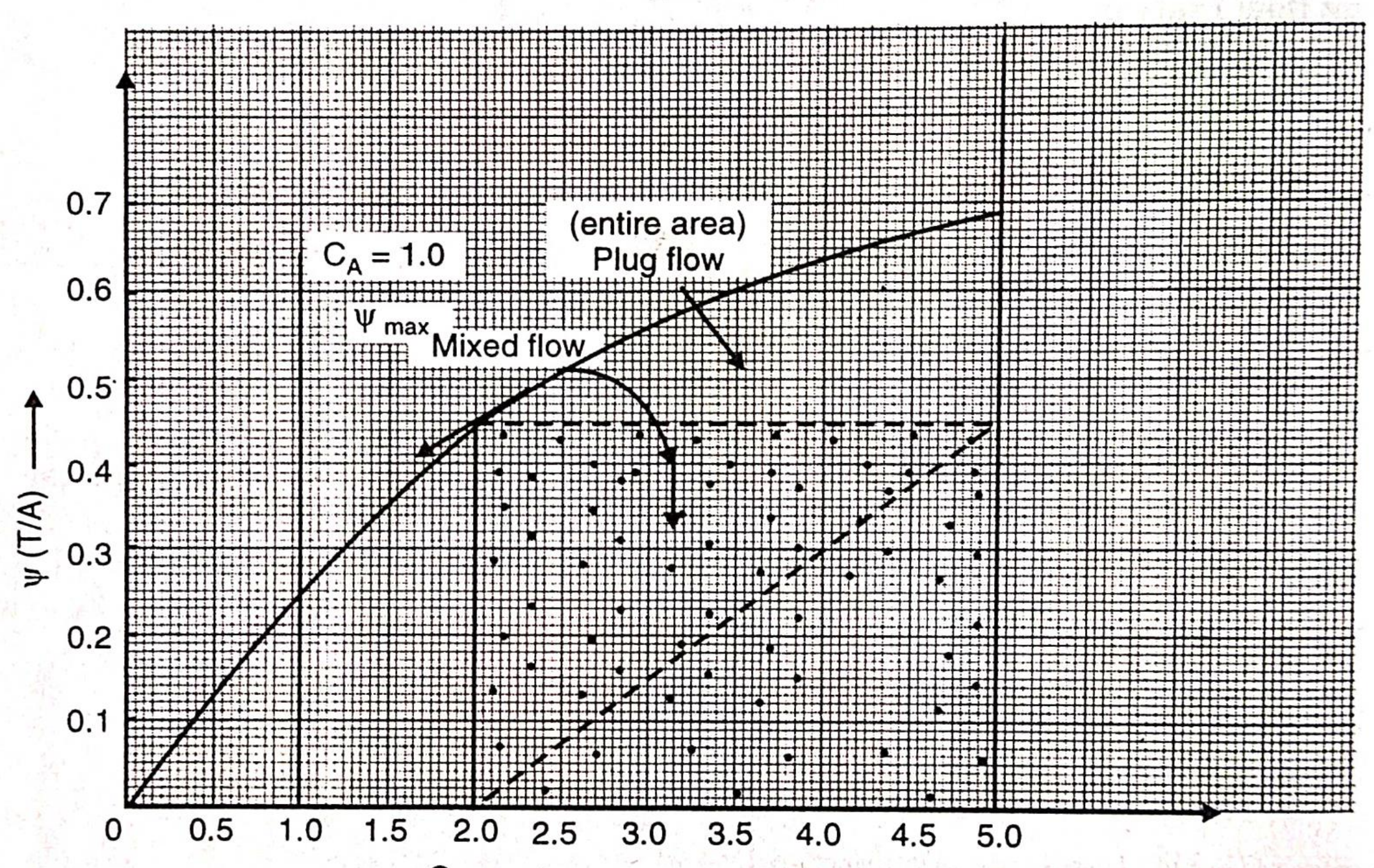
$A \to S$, $r_S = 2\,C_A$

$A \to T$ (desired), $r_T = C_A^2$

$$\varphi(T/A) = \frac{dC_T}{dC_R + dC_S + dC_T} = \frac{C_A^2}{1 + 2C_A + C_A^2}$$

C_A	0	0.5	1	1.5	2	2.5
$\varphi(T/A)$	1	0.11	0.25	0.36	0.44	0.51

C_A	3	3.5	4	4.5	5	
$\varphi(T/A)$	0.56	0.60	0.64	0.67	0.694	



Plug flow reactor:

C_{Af} =0, area is maximum, C_{Tf} = 2.24 mol/Lit (from area under the graph)

- For analytical method in case PFR
- $C_{Sf} = -\int_0^5 \frac{C_A^2}{(1+C_A)^2} dC_A$
- $\int_1^3 \frac{(x-1)^2}{(x)^2} dx = 2\left[(x)_1^6 - 2(lnx)_1^6 - \left(\frac{1}{x}\right)_1^6\right] = 2.25$

Mixed flow reactor:

Area of the rectangle for C_A =2 to C_{A0} =5 is 1.33 mol/lit

Second method: $\emptyset_m$ is maximum for C_A =2

$C_T = \frac{C_A^2}{(1+C_A)^2}(5-2) = \frac{(2)^2}{(3)^2}(3)$ =1.33 mol/Lit

Extra Problem

Q.1 Substance A in a liquid reacts to produce R and S as follows:

$$A \begin{array}{l} \nearrow R \quad \cdots \text{first order} \\ \searrow S \quad \cdots \text{first order} \end{array}$$

A feed ($C_{A0} = 1$, $C_{R0} = 0$, $C_{S0} = 0$) enters two mixed reactors in series ($\tau_1 = 2.5$ min, $\tau_2 = 5$ min). Knowing the composition in the first reactor ($C_{A1} = 0.4$, $C_{R1} = 0.4$, $C_{S1} = 0.2$), find the composition leaving the second reactor.