BT209

Bioreaction Engineering

27/03/2023

Problem 1

Substance A in the liquid phase decomposes as follows:

$$A \rightarrow R \quad r_R = k_1 C_A^2 \quad k_1 = 0.4 \frac{m^3}{mol.\,min}$$

$$A \rightarrow S \quad r_S = k_2 C_A \quad k_2 = 2\ min^{-1}$$

The feed $(C_{A0} = 40,\ C_{R0} = 0, C_{S0} = 0)$ enters a reactor, decomposes and a mixture of A,R and S leaves.

(a) Find the $C_{R,}\ C_s$ and τ for $X_A = 0.9$ in a mixed flow reactor (CSTR)

(b) Find the $C_{R,}\ C_s$ and τ for $X_A = 0.9$ in a Plug flow reactor (PFR)

(c) Find the operating condition (X_A , τ and C_R) which maximize the C_R in a mixed flow reactor

solution

16-2

(a) $$\phi\left(\frac{R}{A}\right) = \frac{0.4\,C_A^2}{0.4\,C_A^2 + 2C_A} = \frac{0.4\times4^2}{0.4\times4^2+2\times4} = \frac{6.4}{14.4}$$

$$\phi\left(\frac{S}{A}\right) = \frac{2C_A}{0.4\,C_A^2 + 2C_A} = \frac{2\times4}{0.4\times4^2+2\times4} = \frac{8}{14.4}$$

$C_{A0} = 40$
$X_A = 0.9$
$\therefore C_A =$

$C_{A0} = 40 \rightarrow \boxed{} \rightarrow C_A = 4$

CSTR

$$C_R = \phi\left(\frac{R}{A}\right)(-\Delta C_A)$$
$$= \frac{6.4}{14.4}\times(40-4) = 16\ \frac{mol}{m^3}$$

$$C_S = \phi\left(\frac{S}{A}\right)(-\Delta C_A)$$
$$= \frac{8}{14.4}(40-4) = 20\ \frac{mol}{m^3}$$

(b) PFR $$\frac{\tau}{C_{A0}} = \frac{X_A}{-r_A} = \frac{0.9}{0.4\,C_A^2+2C_A} = \frac{0.9}{0.4\times4^2+2\times4} = \frac{0.9}{14.4}$$

$$\therefore \tau = 40\times\frac{0.9}{14.4} = 2.5\ min$$

(b) PFR

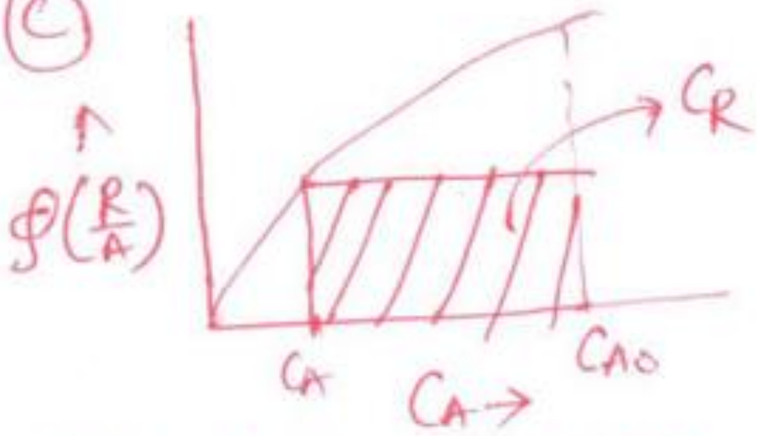
$$C_R = \int_{C_A}^{C_{A0}} \varphi\left(\frac{R}{A}\right) dC_A = \int_4^{40} \frac{0.4 C_A^2}{0.4 C_A^2 + 2 C_A} dC_A = 27.953 \ \frac{mol}{m^3}$$

$$C_S = \int_{C_A}^{C_{A0}} \varphi\left(\frac{S}{A}\right) dC_A = \int_4^{40} \frac{2 C_A}{0.4 C_A^2 + 2 C_A} dC_A = 8.047 \ \frac{mol}{m^3}$$

$$\frac{\tau}{C_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A} = \frac{1}{-C_{A0}} \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A} = \frac{1}{C_{A0}} \int_{C_A}^{C_{A0}} \frac{dC_A}{0.4 C_A^2 + 2 C_A}$$

$$\therefore \tau = \int_4^{40} \frac{dC_A}{0.4 C_A^2 + 2 C_A} = 0.347 \ min$$

(c)



Here C_A is the variable.

For max $C_R = f\left(\frac{R}{A}\right)(-\Delta C_A)$

$$= \frac{0.4\,C_A^2}{0.4\,C_A^2 + 2C_A}\left(C_{A0} - C_A\right)$$

$\Leftarrow$ CSTR $\Rightarrow$ For max C_R, $\frac{dC_R}{dC_A} = 0$

$C_A = 10$

$\therefore C_R = 20$

$$\tau = \frac{C_{A0} X_A}{-r_A} = \frac{40 \times 0.75}{0.4 \times 10^2 + 2 \times 10} = \frac{1}{2}\ \text{min}$$

* $\boxed{\text{method 2} \Rightarrow \text{Area maximization}}$

Problem 2

In a process stream (v = 1 m^3/min) reactant A (C_{A0} = 2) decomposes as follows.

$$
A \begin{cases} \nearrow R & r_R = 1 \\ \rightarrow S & r_S = 2C_A \\ \searrow T & r_T = C_A^2 \end{cases}
$$

Find the maximum expected Cs for isothermal operation

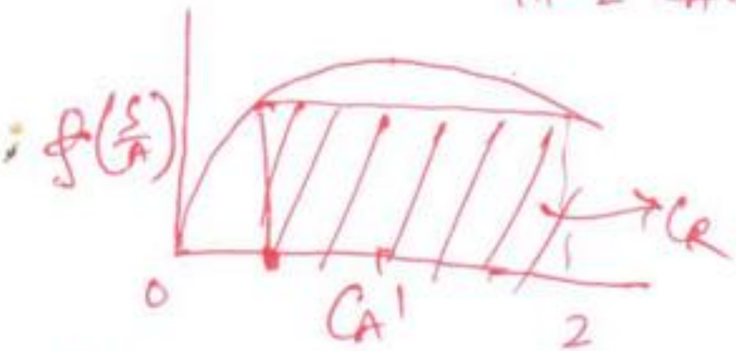
a) in a mixed flow reactor

b) in a plug flow reactor

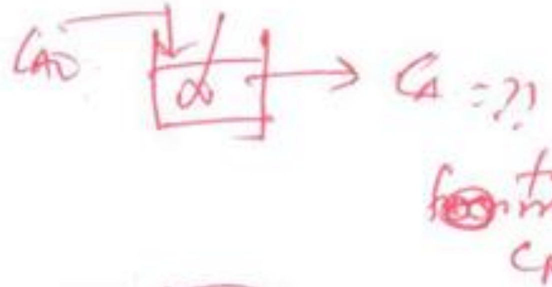
c) in a reactor of your choice if untreated A can be separated from product stream and returned to the feed at C_{A0}=2.

d) any arrangement of reactor where recycle and re-concentration of unreacted feed is not possible

a) $f\left(\frac{S}{A}\right) = \frac{2C_A}{1+2C_A+C_A^2} = \frac{2C_A}{(1+C_A)^2}$



plot $f\left(\frac{S}{A}\right)$ vs C_A



For CSTR

$C_R = f\left(\frac{S}{A}\right)(C_{A0}-C_A)$

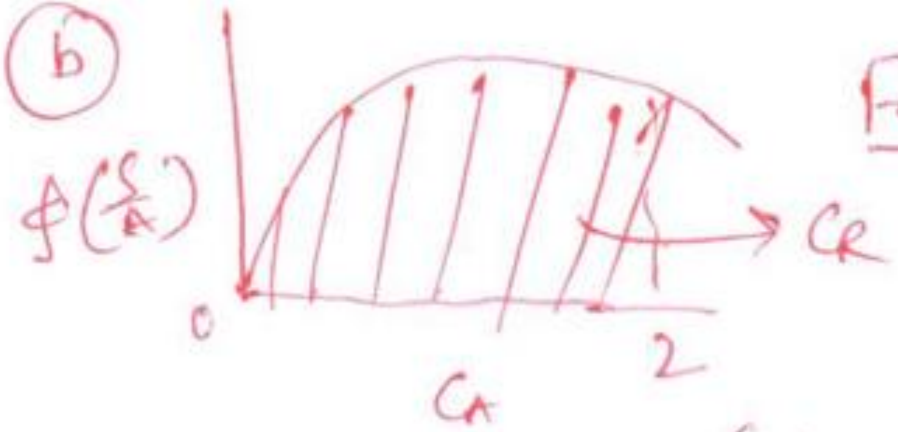
For max C_R

$\frac{dC_R}{dC_A} = 0 \Rightarrow$

$\Downarrow$

$C_A = \frac{1}{2}, \therefore C_S = \frac{2}{3}$

(b)

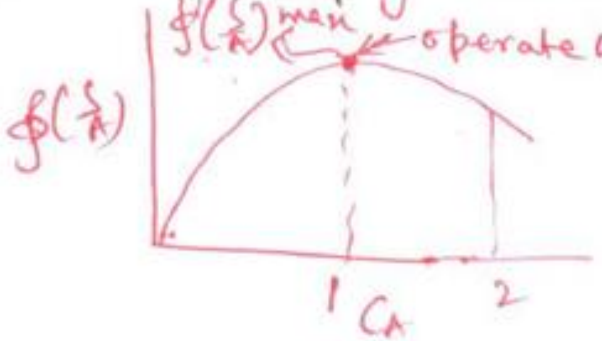


For PFR

C_R (shaded area) is maximum at $C_A \approx 0$ (outlet A)

$$\therefore C_S = -\int_{C_{A0}}^{C_{Af}} f\left(\frac{S}{A}\right) dC_A = \int_0^2 \frac{2C_A}{(1+C_A)^2}\, dC_A = 0.867$$

(c) So running the reactor at the highest $\phi\left(\frac{S}{A}\right)$



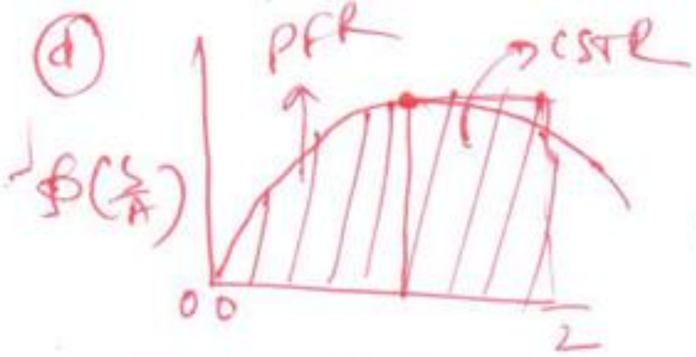
put $\dfrac{d\,\phi\left(\frac{S}{A}\right)}{dC_A} = 0 \Rightarrow C_A = 1$

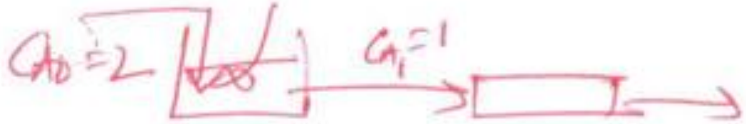
$\phi\left(\frac{S}{A}\right) = 0.5$ (max)

From graph $\Rightarrow$ CSTR is better

$\therefore C_S = \phi\left(\frac{S}{A}\right)(-\Delta C_A) = 0.5 \times (2-1) = 0.5\ \frac{mol}{L}$

(d)





For CSTR $\Rightarrow C_{A0} = 2,\ C_A = 1,\ \therefore C_S = \phi\left(\frac{S}{A}\right)(-\Delta C_A) = 0.5\ \frac{mol}{L}$

For PFR $\Rightarrow C_S = -\int_1^0 \phi\left(\frac{S}{A}\right) dC_A = \int_0^1 \frac{2C_A}{(1+C_A)^2}\, dC_A = 0.386\ \frac{mol}{L}$

Total $C_S = 0.5 + 0.386 = 0.886$ mol/L

Problem 3

In a process stream (v = l m³/min) reactant A (C_{A0} = 10 kmol/m³) decomposes as follows.

$$A \rightarrow R \qquad r_R = 16C_A^{0.5} \quad kmol/m^3/min$$

$$A \rightarrow S \qquad r_S = 12C_A \quad kmol/m^3/min$$

$$A \rightarrow T \qquad r_T = C_A^2 \quad kmol/m^3/min$$

We wish to design a reactor setup for a specific duty. Sketch the scheme selected, and calculate the fraction of feed transformed into desired product as well as the volume of reactor needed.

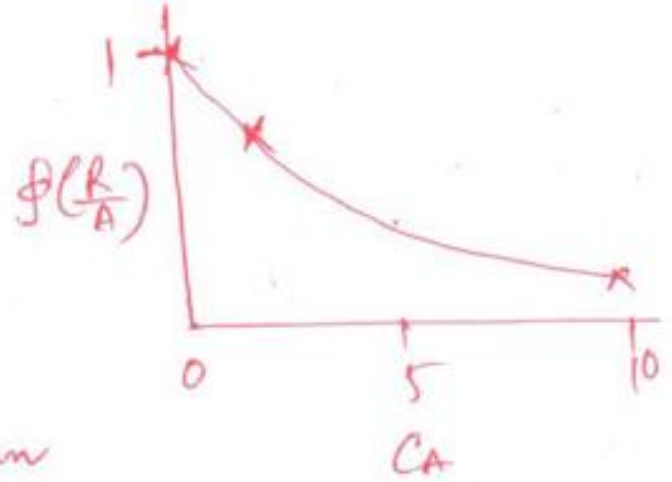
i) When product R is the desired material

ii) When product T is the desired material

T-6-3

(a) $\varphi\left(\frac{R}{A}\right) = \frac{16C_A^{0.5}}{16C_A^{0.5} + 12C_A + C_A^2} = \frac{1}{1 + \frac{12}{16}C_A^{0.5} + \frac{1}{16}C_A^{3/2}}$

C_A	$\varphi\left(\frac{R}{A}\right)$
10	0.185
1	0.55
0	1



at $C_A = 0$, $\varphi\left(\frac{R}{A}\right)$ is maximum

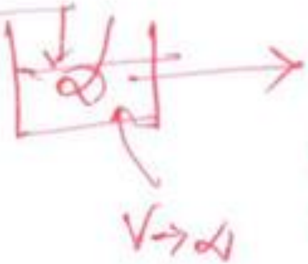
From the graph $\Rightarrow$ CSTR is better than PFR

So, operate the CSTR at $C_A \to 0$ or $X_A \to 1$

$C_{A0} = 10$

$C_{R0} = 0$

$C_{S0} = 0$



$\to C_A = 0$

$C_R = 10$

$C_S = 0$

$$\left\{ \begin{aligned} C_R &= \varphi\left(\tfrac{R}{A}\right)(-\Delta C_A) \\ &= 1 \times (10 - 0) = 10 \end{aligned} \right.$$

$$\frac{\tau}{C_{A0}} = \frac{10-0}{10(16C_A^{1/2} + 12C_A + C_A^2)} = \frac{10}{10} = \alpha$$

$\therefore V = \alpha$

(b) $f\left(\frac{T}{A}\right) = \frac{C_A^2}{16C_A^{1/2} + 12C_A + C_A^2}$

C_A	$f\left(\frac{T}{A}\right)$	$\frac{1}{-r_A}$
10	0.37	0.0037
9	0.39	0.0042
4	0.167	0.0109
1	0.03	0.03
0.1		0.16
0.0001	-	

From graph ⇒ PFR is better

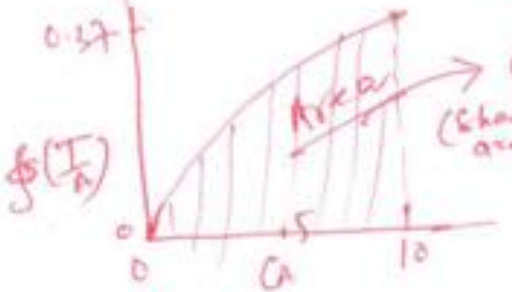
Here, if we rewrite

$f\left(\frac{T}{A}\right) = \frac{1}{16C_A^{-3/2} + 12C_A^{-1} + 1}$

at $C_A = 0$, $f\left(\frac{T}{A}\right) \approx 1$

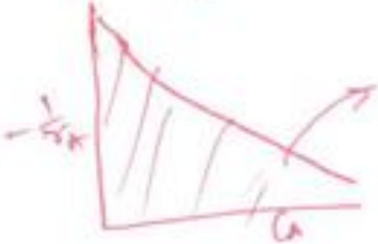
not true

as $C_A \downarrow$ $f\left(\frac{T}{A}\right) \downarrow$



$C_R = \int_{C_{A0}}^{C_A \to \text{close to } 0} f\left(\frac{T}{A}\right) dC_A$ (shaded area)

area $= 2 \frac{mol}{Liter}$



Area $= \tau = \int_{10}^{C_A (\text{close to } 0)} \frac{dC_A}{-r_A}$

$= 0.16$

$\therefore V = \tau v = 0.16 \times 1 = 0.16\ m^3$

$= 160$ liter