1. When aqueous A and aqueous B ($C_{Ao} = C_{Bo}$) are brought together they react in two possible ways:

$$A+B \nearrow R+T, \qquad r_R = 50C_A \text{ mol/m3.hr}$$

$$A+B \searrow S+U, \qquad r_S = 100C_B \text{ mol/m3.hr}$$

to give a mixture whose concentration of active components (A, B, R, S, T, U) is $C_{TOTAL} = C_A + C_B, = 60$ mol/m^3. Find the size of reactor needed and the R/S ratio produced for 90% conversion of an equimolar feed of $F_{Ao} = F_{Bo} =$ 300 mol/hr:

1.1. in a mixed flow reactor;
1.2. in a plug flow reactor;
1.3. which reactor gives more C_R.

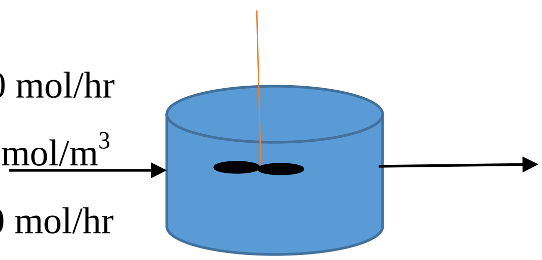
sol.

1.1. $F_{Ao} = 300$ mol/hr

$C_{Ao} = 30$ mol/m^3

$F_{Bo} = 300$ mol/hr

$C_{Bo} = 30$ mol/m^3



$C_A = 3$ mol/m^3

$C_B = 3$ mol/m^3

$$\phi(R/A) = \frac{50\,CA}{50\,CA+100\,CB} = 1/3$$

$$\phi\,(S/A) = \frac{100\,CB}{50\,CA+100\,CB} = 2/3$$

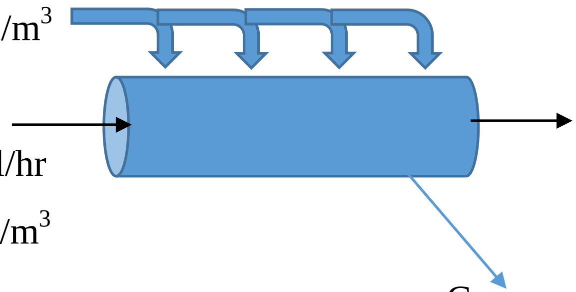
$C_R = \phi\,(R/A) *(-\Delta C_A) = (30-3)/3 = 9$ mol/m^3

R/S = ½

$$V = \frac{FAo}{CAo} \cdot \frac{CAo - CA}{50\,CA+100\,CB} = (300/30)*[(30-3)/(150+300)] = 0.6 \text{ m}^3 = 600 \text{ Lt.}$$

1.2. $F_{Ao} = 300$ mol/hr

$C_{Ao} = 30$ mol/m^3



$C_A = 3$ mol/m^3

$F_{Bo} = 300$ mol/hr

$C_{Bo} = 30$ mol/m^3

$C_{Beverywhere} = C_{Bf} = 3$mol/m^3

$$\phi(R/A) = \frac{50\,CA}{50\,CA+100\,CB}$$

$$\phi\,(S/A) = \frac{100\,CB}{50\,CA+100\,CB}$$

$$C_{Rf} \;=\; \int_{CAf}^{CAo} \phi\left(\frac{R}{A}\right) dCA \;=\; \int_{3}^{30} \frac{CA}{CA+2CB}\, dCA \;=\; 18.68$$

$$C_{Sf} \;=\; \int_{CAf}^{CAo} \phi\left(\frac{S}{A}\right) dCA \;=\; \int_{3}^{30} \frac{2CB}{CA+2CB}\, dCA \;=\; 8.32$$

$$C_{Rf}\,/C_{sf} = 18.68/8.32 = 2.25 \text{ (approx.)}$$

$$V = \frac{FAo}{CAo}\int_{CAf}^{CAo} \frac{dCA}{-rA} \;=\; \frac{300}{30}\int_{30}^{300} \frac{dCA}{50CA+100(3)} = 277.3 \text{ Lt.}$$

1.3. PFR gives more R than CSTR.

2. The elementary liquid-phase-series reaction

$$A \xrightarrow{K_1} B \xrightarrow{K_2} C$$

is carried out in a 500-dm^3 batch reactor. The initial concentration of A is 1.6 mol/dm^3. The desired product is B. and separation of the undesired product C is very difficult and costly. Because the reaction is carried out at a relatively high temperature, the reaction is easily quenched.

$K_1 = 0.4\ h^{-1}$

$K_2 = 0.01\ h^{-1}$ at 100°C

a) Assuming that each reaction is irreversible, plot the concentrations of A, B and C as a function of time.

(b) For a CSTR space time of 0.5 h, what temperature would you recommend to maximize B? (E_1 = 10,000 cal/mol, E_2 = 20,000 cal/mol)

(c) Assume that the first reaction is reversible with $K_{-1} = 0.3\ h^{-1}$. Plot the concentrations of A, B and C as a function of time.

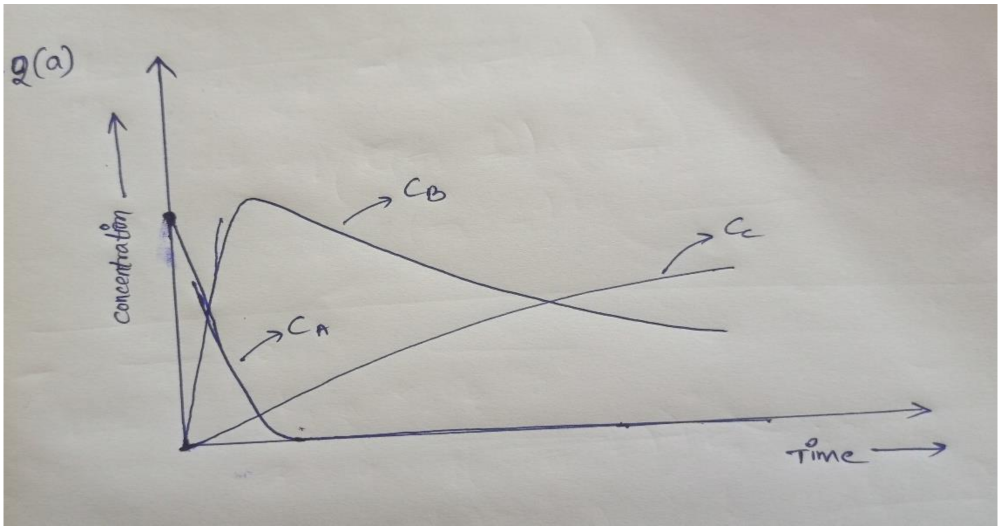
(d) Plot the concentrations of A, B and C as a function of time for the case where both reactions are reversible with $K_{-2} = 0.005\ h^{-1}$.

(e) Vary K_1, K_2, K_{-1} and K_{-2}. Explain the consequence of $K_1 > 100$ and $K_2 < 0.1$ with $K_{-1} = K_{-2} = 0$ and with $K_{-2} = 1$, $K_{-1} = 0$. And $K_{-2} = 0.25$.

Sol. a) Species A: $\frac{dCA}{dt} = rA$; $-r_A = K_1C_A$

Species B: $\frac{dCA}{dt} = rB$; $r_B = K_1C_A - K_2C_B$

Species C: $\frac{dCc}{dt} = rc$; $-r_c = K_2C_B$



b) For CSTR, $\tau = 0.5$ h

First calculate k_1 and k_2:

$$K = Ko\left[\exp\left(\left(\frac{E}{R}\right)\left(\frac{1}{To} - \frac{1}{T}\right)\right)\right]$$

$$K_1 = 0.4\left[\exp\left(\left(\frac{10{,}000}{R}\right)\left(\frac{1}{373} - \frac{1}{T}\right)\right)\right]$$

$$K_2 = 0.01\left[\exp\left(\left(\frac{20{,}000}{R}\right)\left(\frac{1}{373} - \frac{1}{T}\right)\right)\right]$$

$C_A = C_{Ao}e^{-K1}t$

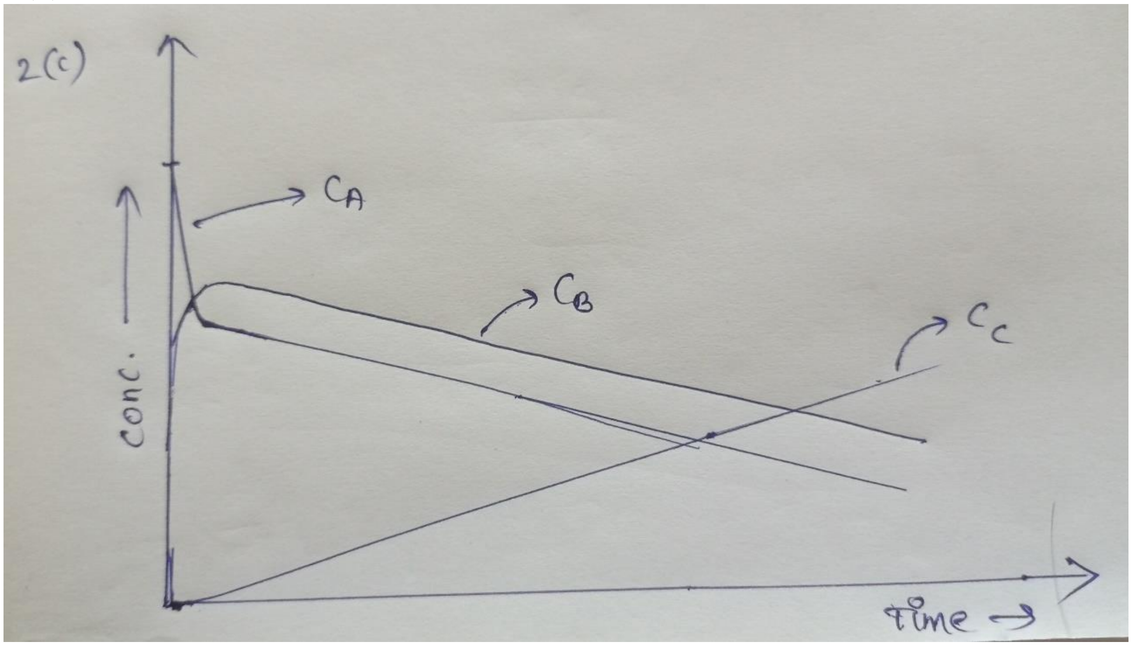
$r_B = K_1C_{Ao}e^{-K1t} - K_2C_B = dC_B/dt$

solving this equation for C_B gives

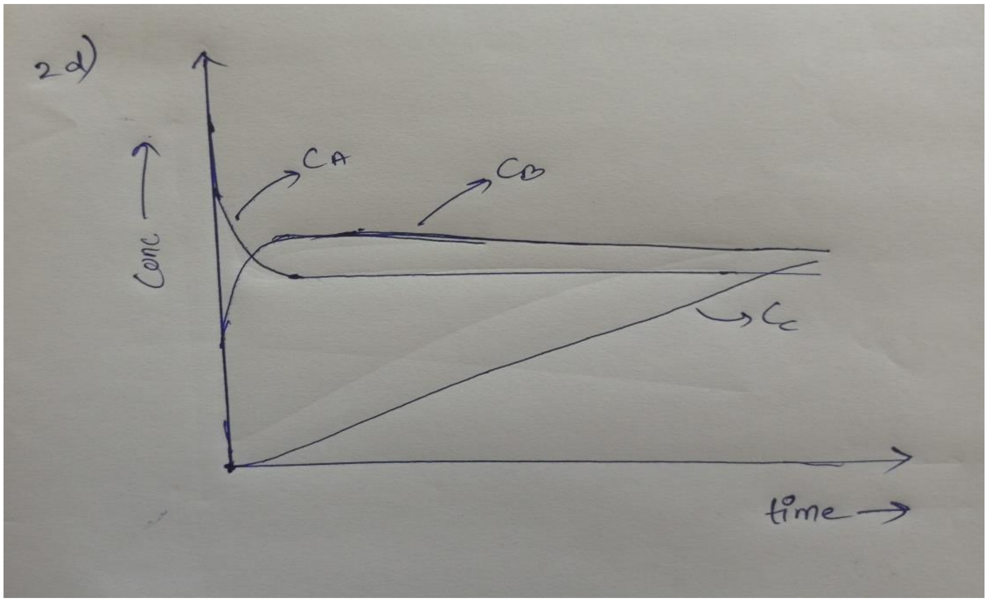
$$C_B = \frac{K1CAo}{K2-K1}(e^{-K1t} - e^{-K2t})$$

On soving $dC_B/dt = 0$ gives that C_B is maximum at T = 760 K.

2(c)



2(d)



e) When K_1>l00 and K_2 < 0.1 the concentration of B immediately shoots up to 1.6 and then slowly comes back down, while C_A drops off immediately and falls to zero. This is because the first reaction is so fast and the second reaction is slower with no reverse reactions.

When k_2 = 1 then the concentration of B spikes again and remains high, while very little of C is formed. This is because after R is formed it will not go to C because the reverse reaction is faster.

when k_{-2} = 0.25, B shoots up, but does not stay as high because the second reverse reaction is a slightly slower than seen before, but still faster than the forward reaction.

3. The elementary liquid phase series parallel reaction scheme

$$A \longrightarrow B \longrightarrow C$$

$$A \longrightarrow R$$

is to be carried out in an isothermal CSTR. The rate laws are given by

$$r_R = k'C_A$$

$$r_B = kC_A - kC_B$$

Feed is pure A. Find the space time of the CSTR which results in the maximum exit concentration of B.

Sol. based on the given reactions, we can write

$$-r_A = kC_A + k'C_A$$

Material balance on A gives:

$$Ʊ_oC_{Ao} = Ʊ_oC_A + (-r_A)V$$

$$C_{Ao} = C_A + (-r_A)\tau_m \qquad (tm = \tau_m = V/Ʊ_o)$$

$$\frac{CA}{CAo} = \frac{1}{1+(k+k')\mathrm{tm}} \ldots\ldots (1)$$

Material balance on B gives:

$$Ʊ_oC_{Bo} = Ʊ_oC_B + (-r_B)V \qquad (\text{since } C_{Bo}=0)$$

$$Ʊ_oC_B = -(-r_B)V \qquad (tm = \tau_m = V/Ʊ_o)$$

$$C_B = \tau_m (kC_A - kC_B)$$

$$C_B = \frac{ktmCA}{1+k\mathrm{tm}} \qquad \ldots\ldots.. (2)$$

Using equation (1) and (2), we get

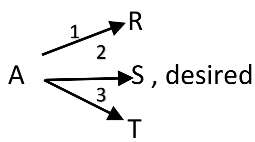
$$\frac{CB}{CAo} = \frac{ktm}{(1+ktm)(1+ktm+k'tm)}$$

Differentiating CB w.r.t. τ_m and equating it to zero gives the optimum τ_m value.

$$d/d\,\tau_m\,(C_B/C_{Ao}) = 0$$

$$\tau_m = \frac{1}{\sqrt{k(k+k')}} \quad .$$

4. For a given feed stream having C_{Ao} should we use a PFR or a MFR and should we use a high or low or some intermediate conversion level for the exit stream if we wish to maximize ϕ(S/A)? The reaction system is



where n_1, n_2, and n_3, are the reaction orders of reactions 1, 2, and 3.

(a) $n_1 = 1$, $n_2 = 2$, $n_3 = 3$

(b) $n_1 = 2$, $n_2 = 3$, $n_3 = 1$

(c) $n_1 = 3$, $n_2 = 1$, $n_3 = 2$

Sol. a) Use a MFR, with a particular concentration of A

b) Use a PFR, with low x_A

c) Use a MFR, with high x_A