

Question Bank 2:
Design of ideal PFRs and ideal CSTRs
operated at steady state under isothermal conditions

Solution to Q1:

Design equation for reactant A in an ideal CSTR operated at steady state is given by

$$F_{A0} = F_{Af} + (-r_A|_{exit}) V \quad (6.1)$$

Since the reaction $A \rightarrow 5R$ is a non-elementary reaction, we could write the rate equation as

$$r_A = -k(C_A)^n \quad (6.2)$$

a) Equation (6.1) gives

$$\begin{aligned} -r_A|_{exit} &= \frac{F_{A0} - F_{Af}}{V} = \frac{F_{A0} x_{Af}}{V} \quad \text{since } F_{Af} = F_{A0}(1 - x_{Af}) \\ &= \frac{v_0 C_{A0} x_{Af}}{V} \quad \text{since } C_{A0} = \frac{F_{A0}}{v_0} \end{aligned} \quad (6.3)$$

To obtain the expression asked for in the question statement, we need to write x_{Af} in terms of concentrations of A at the inlet (C_{A0}) and at the exit (C_{Af}). To get there, we follow the following procedure:

$$x_{Af} \equiv \frac{F_{A0} - F_{Af}}{F_{A0}} = \frac{v_0 C_{A0} - v_f C_{Af}}{v_0 C_{A0}} = 1 - \frac{v_f C_{Af}}{v_0 C_{A0}} \quad (6.4)$$

For a gas-phase reaction, by combining the stoichiometric relationship with the ideal gas equation, we get

$$v_f = \frac{P_0}{P_f} \frac{T_f}{T_0} v_0 (1 + \epsilon_A x_A)$$

where

$$\epsilon = \frac{F_{A0}}{F_{T0}} \left[\frac{(p + q + s + \dots) - (a + b + c + \dots)}{a} \right] = 1 * \left[\frac{5 - 1}{1} \right] = 4$$

Since P and T remain constants, the above expression reduces to

$$v_f = v_0(1 + 4x_{Af}) \quad (6.5)$$

Combining (6.4) and (6.5), we get

$$x_{Af} = 1 - \frac{(1 + 4x_{Af}) C_{Af}}{C_{A0}}$$

which can be rearranged to obtain

$$x_{Af} = \frac{C_{A0} - C_{Af}}{C_{A0} + 4C_{Af}} \quad (6.6)$$

Combining (6.3) and (6.6), we get

$$-r_A|_{exit} = \frac{v_0 C_{A0} x_{Af}}{V} = \frac{v_0 C_{A0}}{V} \left(\frac{C_{A0} - C_{Af}}{C_{A0} + 4C_{Af}} \right) \quad (6.7)$$

b) Reaction order could be determined starting from (6.2). Let us take the natural logarithm of (6.2) to get the following:

$$\ln(-r_A|_{exit}) = n \ln(C_{Af}) + \ln(k) \quad (6.8)$$

Equation (6.7) could be used to determine $(-r_A|_{exit})$ for each of the four runs for which C_{Af} values are known. And, hence, $y = \ln(-r_A|_{exit})$ and $x = \ln(C_{Af})$ could be calculated for all four runs as tabulated below.

Run number	v_0 litre/hr	C_{Af} millimol/litre	$-r_A _{exit}$ millimol/litre.hr	$y = \ln(-r_A _{exit})$	$x = \ln(C_{Af})$
1	3	16	1536.58	7.3373	2.7726
2	10	30	3181.82	8.0652	3.4012
3	30	50	5000	8.5172	3.9120
4	50	60	5882.35	8.6797	4.0943

Plot of y versus x , attached as Set6FigQ1b, shows that the data can be fitted by the straight line $y = 1.0113 x + 4.5648$ which has an $R^2 = 99.51\%$. From which, we get the following:

$n = \text{slope} = 1.0113 \approx 1$ (That is, the given reaction is first-order in A).

$k = \exp(\text{intercept}) = \exp(4.5648) = 96.04$ per hr = 1.60 per min.

c) Equations (6.1), (6.2) and (6.3) are valid for the liquid-phase reaction as well. However, since $v_f \approx v_0$ for a liquid-phase reaction, (6.4) reduces to

$$x_{Af} = 1 - \frac{C_{Af}}{C_{A0}} \quad (6.9)$$

Combining (6.3) and (6.9), we get

$$-r_A|_{exit} = \frac{v_0 C_{A0} x_{Af}}{V} = \frac{v_0}{V} (C_{A0} - C_{Af})$$

Once the value of reaction rate is calculated using the above expression for each of the four runs tabulated, reaction order could be determined in exactly the same way as in part (b) by plotting $y = \ln(-r_A|_{exit})$ versus $x = \ln(C_{Af})$ tabulated below.

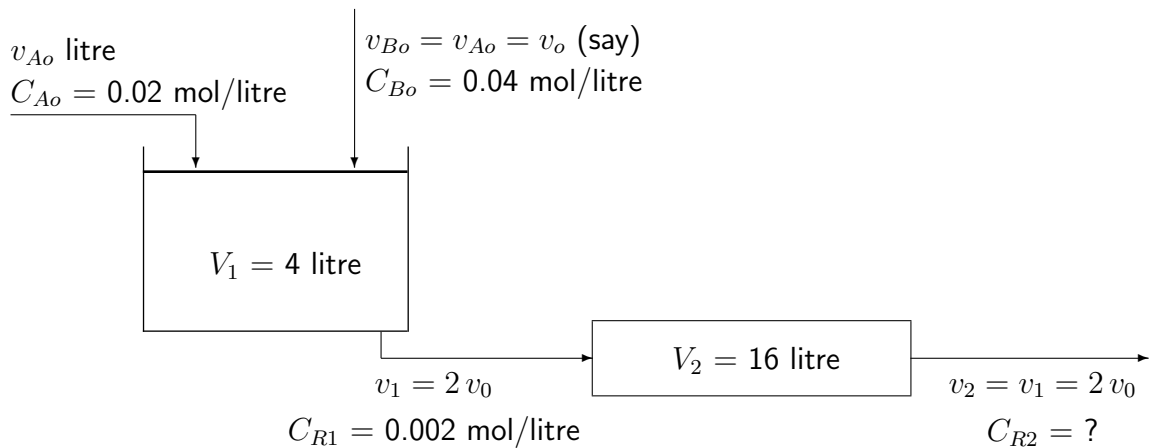
Run number	v_0 litre/hr	C_{Af} millimol/litre	$-r_A _{exit}$ millimol/litre.hr	$y = \ln(-r_A _{exit})$	$x = \ln(C_{Af})$
1	3	16	2520	7.8320	2.7726
2	10	30	7000	8.8537	3.4012
3	30	50	15000	9.6158	3.9120
4	50	60	20000	9.9035	4.0943

Plot of y versus x , attached as Set6FigQ1c, shows that the data can be fitted by the straight line $y = 1.5616 x + 3.5155$, having an $R^2 = 99.96\%$. From which, we get the following:

$$n = \text{slope} = 1.56 \approx 1.5$$

$$k = \exp(\text{intercept}) = \exp(3.5155) = 33.63 \text{ hr}^{-1}. (\text{millimol/litre})^{-0.5}$$

Solution to Q2:



The elementary liquid-phase reaction $A + B \rightarrow R + S$ gives the following rate equation:

$$-r_A = -r_B = r_R = r_S = k C_A C_B \quad (6.10)$$

a) First consider the CSTR of $V_1 (= 4 \text{ litre})$ volume. Since the exit concentration of the product R is known, write down the design equation for product R in an ideal CSTR operated at steady state as

$$F_{R0} + (r_R|_{CSTR\ exit})(V_1) = F_{R1}$$

Since $F_{R0} = 0$ and $F_{R1} = v_1 C_{R1}$, the above reduces to

$$(r_R|_{CSTR\ exit})(V_1) = v_1 C_{R1} = 2 \times v_o \times 0.002 \quad (6.11)$$

From (6.10), we get

$$r_R|_{CSTR\ exit} = k C_{A1} C_{B1} \quad (6.12)$$

In relating C_{A1} and C_{B1} to C_{R1} , we use the following stoichiometric relationship across the CSTR:

$$F_{A0} - F_{A1} = F_{B0} - F_{B1} = F_{R1}$$

which, in terms of concentration, reduces to the following:

$$v_o C_{A0} - 2 v_o C_{A1} = v_o C_{B0} - 2 v_o C_{B1} = 2 v_o C_{R1}$$

From the above, we get the following:

$$C_{A1} = C_{A0}/2 - C_{R1} = 0.02/2 - 0.002 = 0.008 \text{ mol/litre} \quad (6.13)$$

$$C_{B1} = C_{B0}/2 - C_{R1} = 0.04/2 - 0.002 = 0.018 \text{ mol/litre} \quad (6.14)$$

Combining (6.11) to (6.14), we get the following:

$$k \times (0.008) \times (0.018) \times 4 = 2 \times v_o \times 0.002$$

which reduces to the following relationship between the specific rate constant (k) and the volumetric flow rate of the incoming streams (v_o):

$$k = 6.9444 v_o \quad (6.15)$$

Now consider the PFR of V_2 (= 16 litre) volume. Since the conversion of A is to be determined, write down the design equation for A over an ideal PFR operated at steady state as

$$F_A = F_A + dF_A + (-r_A)dV$$

which gives the following:

$$V_2 = \int dV = - \int_{F_{A1}}^{F_{A2}} \frac{1}{(-r_A)} dF_A$$

Substituting $(-r_A)$ from (6.10) in the above, we get the following:

$$V_2 = - \int_{F_{A1}}^{F_{A2}} \frac{1}{k C_A C_B} dF_A = - \int_{F_{A1}}^{F_{A2}} \frac{(2 v_o)^2}{k F_A F_B} dF_A \quad (6.16)$$

Stoichiometry gives $F_A - F_{A0} = F_B - F_{B0}$ and, therefore, $F_B = F_A - F_{A0} + F_{B0}$. which reduces (6.16) to the following:

$$V_2 = - \int_{F_{A1}}^{F_{A2}} \frac{(2 v_o)^2}{k F_A (F_A - F_{A0} + F_{B0})} dF_A$$

Introducing the definition of conversion of A , x_A , the above expression is reduced to the following:

$$V_2 = \int_{x_{A1}}^{x_{A2}} \frac{(2 v_o)^2}{k (1 - x_A) (-F_{A0} x_A + F_{B0})} dx_A \quad (6.17)$$

Using $F_{A_o} = 0.02v_o$ mols and $F_{B_o} = 0.04v_o$ moles in(6.17) along with the relationship between k and v_o given by (6.15), we get

$$\begin{aligned}
 V_2 &= \int_{x_{A1}}^{x_{A2}} \frac{28.80}{(1-x_A)(2-x_A)} dx_A = 28.80 \int_{x_{A1}}^{x_{A2}} \left[\frac{1}{1-x_A} - \frac{1}{2-x_A} \right] dx_A \\
 &= 28.80 \ln \left[\frac{2-x_A}{1-x_A} \right]_{x_{A1}}^{x_{A2}} = 28.80 \left(\ln \left[\frac{2-x_{A2}}{1-x_{A2}} \right] - \ln \left[\frac{2-x_{A1}}{1-x_{A1}} \right] \right) \\
 &= 28.80 \ln \left[\frac{(2-x_{A2})(1-x_{A1})}{(1-x_{A2})(2-x_{A1})} \right] \tag{6.18}
 \end{aligned}$$

To solve the for x_{A2} using (6.18), we know $V_2 = 16$ litre and we need to know x_{A1} . Since, from (6.13), C_{A1} is known as 0.008 mol/litre, x_{A1} can be calculated as follows:

$$x_{A1} = \frac{F_{A_o} - F_{A1}}{F_{A_o}} = 1 - \frac{F_{A1}}{F_{A_o}} = 1 - \frac{C_{A1} \times 2 \times v_o}{C_{A_o} \times v_o} = 1 - \frac{0.008 \times 2}{0.02} = 0.2 = 20\%$$

Using $V_2 = 16$ litre and $x_{A1} = 0.02$ in (6.18), we get the following:

$$\begin{aligned}
 16 &= 28.80 \ln \left[\frac{(2-x_{A2})(0.8)}{(1-x_{A2})(1.8)} \right] \\
 \frac{2-x_{A2}}{1-x_{A2}} &= \frac{1.8}{0.8} \exp(16/28.80) \\
 x_{A2} &= \frac{3.9215 - 2}{3.9215 - 1} = 0.6577 = 66\%
 \end{aligned}$$

That is, conversion of A over the CSTR is 20% and the overall conversion of A over the combined CSTR and PFR system is 66%.

Concentration of R leaving the PFR is calculated as follows:

$$C_{R2} = \frac{F_{R2}}{2v_o} = \frac{F_{A_o} - F_{A2}}{2v_o} = \frac{F_{A_o}x_{A2}}{2v_o} = \frac{C_{A_o}x_{A2}}{2}$$

Since $C_{A_o} = 0.02$ mol/litre and $x_{A2} = 0.6577$, $C_{R2} = 0.0066$ mol/litre.

b) If the final conversion of A is to be increased by another 10% to $x_{A3} = 76\%$ by introducing an additional PFR, which is to be connected to the outlet of the existing PFR, the volume of the additional PFR required (V_3) for this purpose could be calculated by modifying (6.18) as follows:

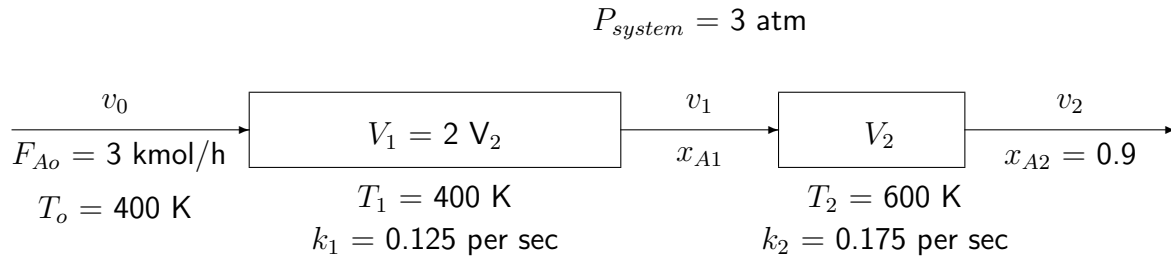
$$V_2 + V_3 = 28.80 \ln \left[\frac{(2-x_{A3})(1-x_{A1})}{(1-x_{A3})(2-x_{A1})} \right]$$

Since $V_2 = 16$ litre and $x_{A1} = 0.2$, we get the following:

$$16 + V_3 = 28.80 \ln \left[\frac{(2-0.76)(1-0.2)}{(1-0.76)(2-0.2)} \right] = 23.94$$

which gives $V_3 = 23.94 - 16 = 7.94$ litre.

Solution to Q3:



The elementary, gas-phase reaction $A \rightarrow B + C$ is carried out in the system shown above. The volumes of the reactors are to be determined. Since the reaction is elementary, we can write the following:

$$-r_A = k C_A = k F_A / v \quad (6.19)$$

where C_A is the concentration of A , F_A is the molar flow rate of A and v is the volumetric flow rate.

Steady-state design equation over the first PFR of V_1 volume gives the following:

$$V_1 = - \int_{F_{Ao}}^{F_{A1}} \frac{1}{(-r_A)} dF_A$$

Using (6.19) and the definition of conversion of A in the above, we get the following:

$$V_1 = - \int_{F_{Ao}}^{F_{A1}} \frac{v}{k F_A} dF_A = \int_{x_{Ao}}^{x_{A1}} \frac{v}{k(1-x_A)} dx_A \quad (6.20)$$

Since it is a gas-phase reaction v is related to x_A by

$$v = \frac{P_o T_1}{P_1 T_o} v_o (1 + \epsilon_A x_A),$$

of which, $P_o = P_1 = 3 \text{ atm}$, $T_o = T_1 = 400 \text{ K}$ and $\epsilon_A = (2-1)/1 = 1$. Therefore, the above expression reduces to

$$v = v_o (1 + x_A) \quad (6.21)$$

Combining (6.20) and (6.21), we get

$$V_1 = \frac{v_o}{k_1} \int_{x_{Ao}}^{x_{A1}} \frac{1 + x_A}{1 - x_A} dx_A \quad (6.22)$$

where k_1 is the specific reaction rate (k) at 400 K.

Steady-state design equation over the second PFR of V_2 volume gives the following:

$$V_2 = - \int_{F_{A1}}^{F_{A2}} \frac{1}{(-r_A)} dF_A = - \int_{F_{A1}}^{F_{A2}} \frac{v}{k F_A} dF_A = \int_{x_{A1}}^{x_{A2}} \frac{v}{k(1-x_A)} dx_A \quad (6.23)$$

In the above, v is related to x_A by

$$v = \frac{P_o T_2}{P_2 T_o} v_o (1 + \epsilon_A x_A),$$

of which, $P_o = P_2 = 3 \text{ atm}$, $T_o = 400 \text{ K}$, $T_2 = 600 \text{ K}$ and $\epsilon_A = 1$. Therefore, the above expression reduces to

$$v = \frac{600}{400} v_o (1 + x_A) \quad (6.24)$$

Combining (6.23) and (6.24), we get

$$V_2 = \frac{600 v_o}{400 k_2} \int_{x_{A1}}^{x_{A2}} \frac{1 + x_A}{1 - x_A} dx_A \quad (6.25)$$

where k_2 is the specific reaction rate (k) at 600 K.

Adding (6.22) multiplied by k_1/v_o to (6.25) multiplied by $400 k_2/600 v_o$, we get the following:

$$\begin{aligned} \frac{k_1}{v_o} V_1 + \frac{400 k_2}{600 v_o} V_2 &= \int_{x_{Ao}}^{x_{A2}} \frac{1 + x_A}{1 - x_A} dx_A \\ &= \int_{x_{Ao}}^{x_{A2}} \left(\frac{2}{1 - x_A} - 1 \right) dx_A \\ &= \left[-2 \ln(1 - x_A) - x_A \right] \Big|_{x_{Ao}=0}^{x_{A2}=0.9} \\ &= -2 \ln(1 - 0.9) - 0.9 = 3.7052 \end{aligned}$$

Using the numerical values of k_1 and k_2 and the information that $V_1 = 2 V_2$ in the above, we get

$$\frac{0.125}{v_o} \times 2 V_2 + \frac{400 \times 0.175}{600 v_o} V_2 = 3.7052$$

which gives

$$V_2 = \frac{3.7052 v_o}{2 \times 0.125 + 4 \times 0.175/6} = (10.1050 \text{ sec}) \times v_o \quad (6.26)$$

The volumetric flow rate at the entrance (v_o) appearing in (6.26) could be determined as follows:

$$v_o = \frac{F_{Ao} R T_o}{P_o} = \frac{(3/3600 \text{ kmol/s}) \times (8.314 \text{ kJ/kmol.K}) \times (400 \text{ K})}{3 \times 1.0132 \times 100 \text{ kPa}} = 0.009117 \text{ m}^3/\text{s}$$

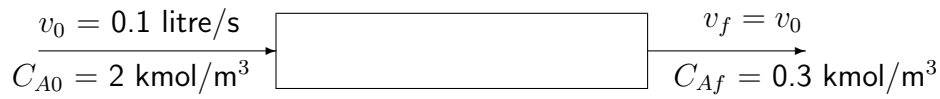
Substituting the above in (6.26), we get $V_2 = 92.13 \text{ litre}$.

Therefore, the volume of the first PFR should be 184.26 litre and the second PFR should be 92.13 litre to achieve 90% overall conversion of A at the exit of the second PFR.

Note:

Solution to Q4 is not provided since it is part of Assignment 2.

Solution to Q5:



The elementary, liquid-phase reactions taking place in the PFR, operated at steady-state under isothermal conditions, are as follows:



where $k_1 = 0.003 \text{ sec}^{-1}$, $k_2 = 0.001 \text{ sec}^{-1}$ and $k_3 = k_2 - k_1$.

a) To determine the space-time of the reactor, let us write the mass balance for reactant A over a differential volume dV of the PFR as follows:

$$F_A = F_A + dF_A + (-r_A)|_{A \rightarrow R} dV \quad (6.27)$$

We deal with liquid-phase reactions and therefore

$$F_A = v_0 C_A. \quad (6.28)$$

The rate equation for the elementary reaction $A \rightarrow R$ is given by

$$(-r_A)|_{A \rightarrow R} = k_1 C_A. \quad (6.29)$$

Combining (6.27) to (6.29), we get

$$v_0 dC_A = -k_1 C_A dV \quad (6.30)$$

which, upon integration, yields the volume of the reactor (V) as follows:

$$V = - \int_{C_{A0}}^{C_{Af}} \frac{v_0}{k_1 C_A} dC_A = -\frac{v_0}{k_1} \ln \left(\frac{C_{Af}}{C_{A0}} \right)$$

Space-time τ defined as the ratio between the volume of the reactor and the volumetric flow rate, therefore, becomes

$$\tau = \frac{V}{v_0} = \frac{1}{k_1} \ln \left(\frac{C_{A0}}{C_{Af}} \right) = \frac{1}{0.003 \text{ sec}^{-1}} \ln \left(\frac{2}{0.3} \right) = 632.4 \text{ sec} = 10.54 \text{ min}. \quad (6.31)$$

b) To determine the concentrations of R and S at the outlet of the reactor, we need to write the mass balances for R and S over the differential volume dV of the PFR. First, let us write the mass balance for R which is a product in the reaction $A \rightarrow R$ and a reactant in the reactions $R \rightarrow 2S$ and $R \rightarrow P$. The mass balance therefore becomes the following:

$$F_R + (r_R)|_{A \rightarrow R} dV = F_R + dF_R + (-r_R)|_{R \rightarrow 2S} dV + (-r_R)|_{R \rightarrow P} dV \quad (6.32)$$

The reaction rates in (6.32) can be written in terms of concentrations as follows:

$$(r_R)|_{A \rightarrow R} = (-r_A)|_{A \rightarrow R} = k_1 C_A \quad (6.33)$$

$$(-r_R)|_{R \rightarrow 2S} = k_2 C_R \quad (6.34)$$

$$(-r_R)|_{R \rightarrow P} = k_3 C_R \quad (6.35)$$

Combining (6.32) to (6.35) along with $F_R = v_0 C_R$, we get

$$k_1 C_A dV = v_0 dC_R + k_2 C_R dV + k_3 C_R dV$$

which can be rearranged, using $\tau = V/v_0$, to give the following:

$$\frac{dC_R}{d\tau} = k_1 C_A - k_2 C_R - k_3 C_R = k_1 C_A - k_2 C_R - (k_1 - k_2) C_R = k_1 C_A - k_1 C_R \quad (6.36)$$

Integrating (6.36) requires C_A be written in terms of C_R or τ . Starting from (6.30), we could get

$$\frac{dC_A}{d\tau} = -k_1 C_A$$

which upon integration, using the initial condition $C_A = C_{A0}$ at $\tau = 0$, gives the following:

$$C_A = C_{A0} e^{-k_1 \tau} \quad (6.37)$$

Combining (6.36) and (6.37), we get

$$\frac{dC_R}{d\tau} + k_1 C_R = k_1 C_{A0} e^{-k_1 \tau} \quad (6.38)$$

which could be integrated as follows:

$$\left(\frac{dC_R}{d\tau} + k_1 C_R \right) e^{k_1 \tau} = k_1 C_{A0} e^{-k_1 \tau} e^{k_1 \tau}$$

$$\frac{d}{d\tau} (C_R e^{k_1 \tau}) = k_1 C_{A0}$$

$$C_R e^{k_1 \tau} = k_1 C_{A0} \tau + const \quad (6.39)$$

Using the initial condition, $C_R = 0$ at $\tau = 0$, (6.39) is reduced to the following:

$$C_R = k_1 \tau C_{A0} e^{-k_1 \tau} \quad (6.40)$$

Writing the mass balance for S which is a product in the reaction $R \rightarrow 2S$, we get the following:

$$F_S + (r_S)|_{R \rightarrow 2S} dV = F_S + dF_S \quad (6.41)$$

The reaction rate in (6.41) can be written as follows:

$$(r_S)|_{R \rightarrow 2S} = 2 \times (-r_R)|_{R \rightarrow 2S} = 2 k_2 C_R \quad (6.42)$$

Combining (6.41) and (6.42) along with $F_S = v_0 C_S$ and $\tau = V/v_0$, we get

$$\frac{dC_S}{d\tau} = 2 k_2 C_R \quad (6.43)$$

Combining (6.40) and (6.43), we get

$$\frac{dC_S}{d\tau} = 2 k_1 k_2 \tau C_{A0} e^{-k_1 \tau} \quad (6.44)$$

which upon integration gives the following:

$$C_S = 2 k_1 k_2 C_{A0} \int \tau e^{-k_1 \tau} d\tau \quad (6.45)$$

To get the integral in (6.45), do the following:

$$\begin{aligned} \frac{d}{d\tau} (\tau e^{-k_1 \tau}) &= e^{-k_1 \tau} + \tau (-k_1 e^{-k_1 \tau}) \\ \int d(\tau e^{-k_1 \tau}) &= \int e^{-k_1 \tau} d\tau - k_1 \int \tau e^{-k_1 \tau} d\tau \\ \tau e^{-k_1 \tau} &= \frac{e^{-k_1 \tau}}{-k_1} - k_1 \int \tau e^{-k_1 \tau} d\tau \\ k_1 \int \tau e^{-k_1 \tau} d\tau &= -\tau e^{-k_1 \tau} - \frac{e^{-k_1 \tau}}{k_1} \end{aligned} \quad (6.46)$$

Combining (6.45) and (6.46), we get

$$C_S = -2 k_2 C_{A0} \left(\tau e^{-k_1 \tau} + \frac{e^{-k_1 \tau}}{k_1} \right) + const$$

which, using the initial condition $C_S = 0$ at $\tau = 0$, is reduced to the following:

$$C_S = -2 k_2 C_{A0} \left(\tau e^{-k_1 \tau} + \frac{e^{-k_1 \tau}}{k_1} - \frac{1}{k_1} \right) \quad (6.47)$$

Using $\tau = 632.4$ sec from (6.31) and the numerical values of k_1 , k_2 and C_{A0} , we can calculate C_R using (6.40) and C_S using (6.47) as follows:

$$C_R = 0.569 \text{ kmol/m}^3 \text{ and } C_S = 0.754 \text{ kmol/m}^3$$

c) To determine the volume of the PFR that maximizes the concentration of R at the outlet for the given conditions, we need to set $dC_R/d\tau = 0$. Using the expression for C_R given in (6.40), we get the following:

$$\frac{dC_R}{d\tau} = \frac{d}{d\tau} (k_1 \tau C_{A0} e^{-k_1 \tau}) = 0$$

which reduces to

$$e^{-k_1 \tau} + \tau (-k_1 e^{-k_1 \tau}) = 0$$

Therefore, the space-time of the PFR that maximizes the concentration of R at the outlet is given by

$$\tau_{optimum} = \frac{1}{k_1} = \frac{1}{0.003} = 333.3 \text{ sec} = 5.56 \text{ min.}$$

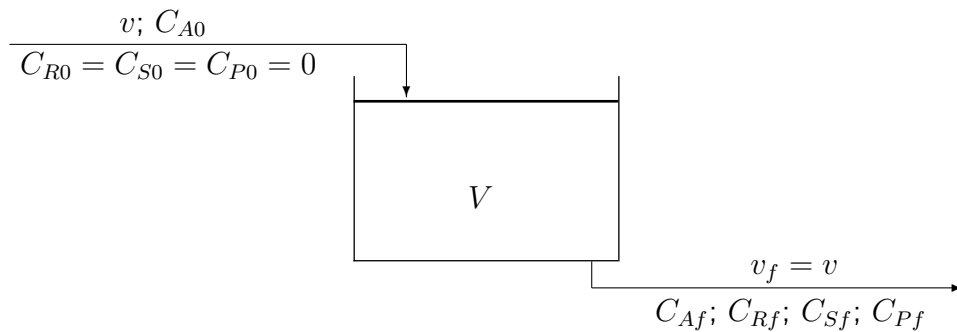
The volume of the PFR that maximizes the concentration of R at the outlet is given by

$$V_{optimum} = v_0 \times \tau_{optimum} = (0.1 \text{ litre/sec}) \times (333.3 \text{ sec}) = 33.33 \text{ litre.}$$

Note:

Solution to Q6 is not provided since it is part of Assignment 2.

Solution to Q7:



The elementary, liquid-phase reactions taking place in the CSTR, operated at steady-state under isothermal conditions, are as follows:



a) To determine the concentration of R in the exit stream, we need to write the mass balance for R over the CSTR. Since R is a product in the reaction $A \rightarrow R$ and a reactant in the reactions $R \rightarrow S$, the mass balance for R over the CSTR becomes the following:

$$v C_{R0} + [(r_R)|_{A \rightarrow R}]_{exit} V = v C_{Rf} + [(-r_R)|_{R \rightarrow S}]_{exit} V \quad (6.48)$$

The reaction rates in (6.53) can be written in terms of the concentrations as follows:

$$[(r_R)|_{A \rightarrow R}]_{exit} = [(-r_A)|_{A \rightarrow R}]_{exit} = 4k C_{Af} \quad (6.49)$$

$$[(-r_R)|_{R \rightarrow S}]_{exit} = k C_{Rf} \quad (6.50)$$

Combining (6.53) to (6.55) and using $C_{R0} = 0$, we get

$$4k C_{Af} V = v C_{Rf} + k C_{Rf} V$$

which gives the following:

$$C_{Rf} = \frac{4k C_{Af} V}{v + k V} = \frac{4k \tau}{1 + k \tau} C_{Af} \quad (6.51)$$

To write C_{Af} of (6.51) in terms of C_{A0} , let us write the mass balance for A over the CSTR as follows:

$$v C_{A0} = v C_{Af} + [(-r_A)|_{A \rightarrow R}]_{exit} V + [(-r_A)|_{A \rightarrow P}]_{exit} V \quad (6.52)$$

The reaction rates in (6.52) can be written in terms of concentrations as follows:

$$[(-r_A)|_{A \rightarrow R}]_{exit} = 4k C_{Af} \quad (6.53)$$

$$[(-r_A)|_{A \rightarrow P}]_{exit} = k C_{Af} \quad (6.54)$$

Combining (6.52) to (6.54), we get

$$v C_{A0} = v C_{Af} + 4k C_{Af} V + k C_{Af} V$$

which gives

$$C_{Af} = \frac{v C_{A0}}{v + 5k V} = \frac{1}{1 + 5k \tau} C_{A0} \quad (6.55)$$

Combining (6.51) and (6.55), we get the following:

$$C_{Rf} = \frac{4k \tau}{(1 + k \tau)(1 + 5k \tau)} C_{A0} \quad (6.56)$$

b) To determine the space-time of the CSTR that maximizes the concentration of R at the exit, we need to set $dC_{Rf}/d\tau = 0$. Using the expression for C_{Rf} given in (6.56), we get the following:

$$\frac{dC_{Rf}}{d\tau} = \frac{d}{d\tau} \left[\frac{4k \tau}{(1 + k \tau)(1 + 5k \tau)} C_{A0} \right] = 0$$

which can be reduced as follows:

$$\begin{aligned} \frac{-5k \tau}{(1 + k \tau)(1 + 5k \tau)^2} + \frac{-k \tau}{(1 + k \tau)^2(1 + 5k \tau)} + \frac{1}{(1 + k \tau)(1 + 5k \tau)} &= 0 \\ -5k \tau (1 + k \tau) - k \tau (1 + 5k \tau) + (1 + k \tau)(1 + 5k \tau) &= 0 \\ -5k \tau - 5(k \tau)^2 - k \tau - 5(k \tau)^2 + 1 + 6k \tau + 5(k \tau)^2 &= 0 \\ (k \tau)^2 &= 1/5 \end{aligned}$$

Therefore, the space-time of the CSTR that maximizes the concentration of R at the exit is given by the following:

$$\tau_{optimum} = \frac{1}{\sqrt{5}k} \quad (6.57)$$

c) For the case of $k = 1 \text{ min}^{-1}$ and $C_{A0} = 2 \text{ kgmol/m}^3$, concentrations of A , R , S and P in the exit stream of the CSTR as functions of τ are to be sketched. Concentrations of A and

R in the exit stream of the CSTR are given by (6.55) and (6.56), respectively. Using $k = 1 \text{ min}^{-1}$ and $C_{A0} = 2 \text{ kgmol/m}^3$, we get the following:

$$C_{Af} = \frac{1}{1 + 5k\tau} C_{A0} = \frac{2}{1 + 5\tau} \text{ kgmol/m}^3 \quad (6.58)$$

$$C_{Rf} = \frac{4k\tau}{(1 + k\tau)(1 + 5k\tau)} C_{A0} = \frac{8\tau}{(1 + \tau)(1 + 5\tau)} \text{ kgmol/m}^3 \quad (6.59)$$

To determine C_{Sf} and C_{Pf} , let us write the mass balances for S and P over the CSTR as follows:

For S :

$$v C_{S0} + [(r_S)|_{R \rightarrow S}]_{exit} V = v C_{Sf} \quad (6.60)$$

where

$$[(r_S)|_{R \rightarrow S}]_{exit} = [(-r_R)|_{R \rightarrow S}]_{exit} = k C_{Rf} \quad (6.61)$$

Combining (6.60) and (6.61) along with $C_{S0} = 0$, we get

$$k C_{Rf} V = v C_{Sf}$$

which gives the following:

$$C_{Sf} = k\tau C_{Rf} \quad (6.62)$$

For P :

$$v C_{P0} + [(r_P)|_{A \rightarrow P}]_{exit} V = v C_{Pf} \quad (6.63)$$

where

$$[(r_P)|_{A \rightarrow P}]_{exit} = [(-r_A)|_{A \rightarrow P}]_{exit} = k C_{Af} \quad (6.64)$$

Combining (6.63) and (6.64) along with $C_{P0} = 0$, we get

$$k C_{Af} V = v C_{Pf}$$

which gives the following:

$$C_{Pf} = k\tau C_{Af} \quad (6.65)$$

Using $k = 1 \text{ min}^{-1}$ in (6.62) and (6.65) and using (6.58) and (6.59), we get the following:

$$C_{Sf} = \frac{8\tau^2}{(1 + \tau)(1 + 5\tau)} \text{ kgmol/m}^3 \quad (6.66)$$

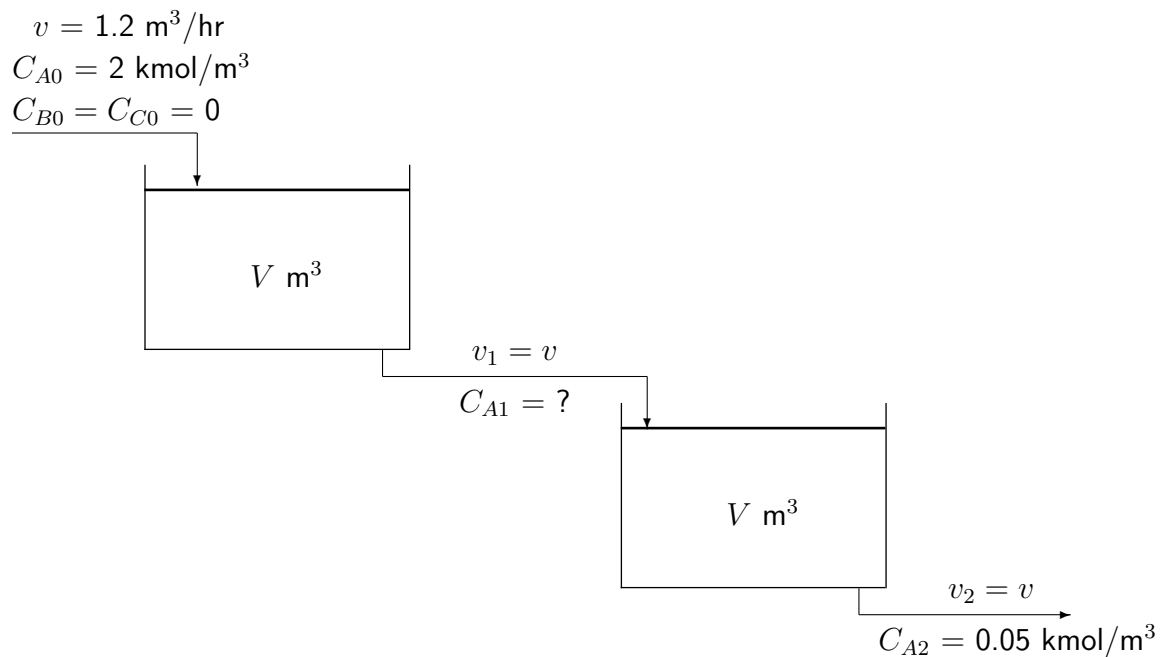
$$C_{Pf} = \frac{2\tau}{(1 + 5\tau)} \text{ kgmol/m}^3 \quad (6.67)$$

Plot of the concentrations as functions of space-time is attached as Set6FigQ7.

Note:

Solution to Q8 is not provided since it is part of Assignment 2.

Solution to Q9:



The liquid-phase reaction taking place in the CSTRs, operated at steady-state under isothermal conditions, is $A \rightarrow 2B + C$, which is first-order in A . Therefore, the rate equation is given by the following:

$$r_A = -kC_A \quad (6.68)$$

where $k = 21$ per hr.

a) To determine the volumes of the CSTRs required and the concentration of A in the exit stream of the first CSTR, we need to write the mass balance for A over the first CSTR as follows:

$$vC_{A0} = vC_{A1} + (-r_A)_{\text{exit of the first CSTR}} V$$

which becomes

$$vC_{A0} = vC_{A1} + kC_{A1}V \quad (6.69)$$

Substituting the known values in the above, we get

$$(1.2 \text{ m}^3/\text{hr}) \times (2 \text{ kmol/m}^3) = (1.2 \text{ m}^3/\text{hr}) \times C_{A1} + (21 \text{ per hr}) C_{A1} V$$

which can be reduced to the following:

$$21C_{A1}V + 1.2C_{A1} = 2.4 \quad (6.70)$$

There are two unknowns in (6.70), and therefore we need a second equation to solve for the unknowns. The second equation may be obtained by writing the mass balance for A over the second CSTR as follows:

$$vC_{A1} = vC_{A2} + kC_{A2}V \quad (6.71)$$

Substituting the known values in the above, we get

$$(1.2 \text{ m}^3/\text{hr}) \times C_{A1} = (1.2 \text{ m}^3/\text{hr}) \times (0.05 \text{ kmol/m}^3) + (21 \text{ per hr}) (0.05 \text{ kmol/m}^3) V$$

which can be reduced to the following:

$$1.2 C_{A1} = 0.06 + 1.05 V \quad (6.72)$$

Combining (6.70) and (6.72) so as to eliminate C_{A1} gives

$$1.2 \times \frac{2.4}{21 V + 1.2} = 0.06 + 1.05 V$$

which reduces to the following:

$$22.05 V^2 + 2.52 V - 2.808 = 0$$

Solving the quadratic equation above gives the volume of a single CSTR as follows:

$$V = \frac{-2.52 \pm \sqrt{(2.52)^2 + 4 \times 22.05 \times 2.808}}{2 \times 22.05} = 0.304 \text{ m}^3$$

Therefore, we require two CSTRs of 0.304 m^3 each to carryout the given reaction.

Substituting $V = 0.304 \text{ m}^3$ in (6.70) gives the concentration of A leaving the first CSTR as follows:

$$C_{A1} = \frac{2.4}{21 V + 1.2} = 0.316 \text{ kmol/m}^3$$

b) If the reactor system of two CSTRs were replaced by one single CSTR, then the mass balance for A over the CSTR gives

$$v C_{A0} = v C_{A2} + (-r_A)_{exit} V_{single\ CSTR}$$

which becomes the following:

$$v C_{A0} = v C_{A2} + k C_{A2} V_{single\ CSTR}$$

Therefore,

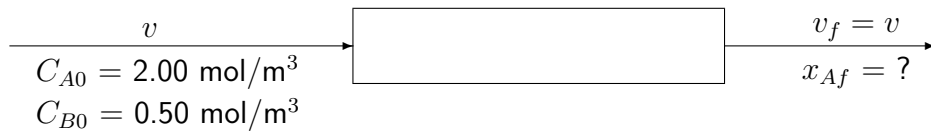
$$V_{single\ CSTR} = \frac{v (C_{A0} - C_{A2})}{k C_{A2}} = \frac{1.2 \times (2 - 0.05)}{21 \times 0.05} = 2.229 \text{ m}^3 \quad (6.73)$$

The volume of the single CSTR, being 2.229 m^3 , is much larger than the total volume of the two CSTRs considered in the part (a), which is 0.608 m^3 , for the same task.

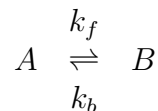
IMPORTANT:

Explanation to why the volume of the single CSTR is larger than the total volume of the two CSTRs for the same task can be given with the help of the $1/(-r_A)$ versus C_A curve attached as Set6FigQ9. Try to explain on your own. Help is provided if required.

Solution to Q10:



The elementary, liquid-phase, reversible reaction taking place in the PFR, operated at steady-state under isothermal conditions, is as follows:



where $k_f = 0.80$ per min and $k_b = 1.20$ per min.

a) To determine the relationship between the conversion of A at the exit, x_{Af} , and the space-time of the PFR, $\tau = V/v$, we need to start with the mass balance for A over a differential volume dV of the PFR. Since A is the reactant in the forward reaction and it is the product in the backward reaction, the said mass balance is written as follows:

$$F_A + (r_A)|_{B \rightarrow A} dV = F_A + dF_A + (-r_A)|_{A \rightarrow B} dV \quad (6.74)$$

The reactions rates in (6.74) are written as follows:

$$(-r_A)|_{A \rightarrow B} = k_f C_A \quad (6.75)$$

$$(r_A)|_{B \rightarrow A} = (-r_B)|_{B \rightarrow A} = k_b C_B \quad (6.76)$$

Combining (6.74) to (6.76), we get

$$k_b C_B dV = dF_A + k_f C_A dV \quad (6.77)$$

which, using $F_A = v C_A$, can be reduced to the following:

$$k_b C_B dV = v dC_A + k_f C_A dV$$

Using the definition of space-time, $\tau = V/v$, the above can be rewritten as follows:

$$(k_b C_B - k_f C_A) d\tau = dC_A \quad (6.78)$$

To integrate (6.78) we need to get rid of the variable C_B from (6.78), which can be done starting from the following stoichiometric relationship between the molar flow rates F_A and F_B :

$$\frac{F_{A0} - F_A}{1} = \frac{F_B - F_{B0}}{1}$$

Dividing the above by the volumetric flow rate, we get

$$C_{A0} - C_A = C_B - C_{B0}$$

which can be rewritten as follows:

$$C_B = C_{A0} + C_{B0} - C_A \quad (6.79)$$

Combining (6.78) and (6.79), we get

$$[k_b (C_{A0} + C_{B0}) - (k_b + k_f) C_A] d\tau = dC_A$$

which, by substituting the variables with the numerical values provided, is reduced to the following:

$$[1.20 (2.00 + 0.50) - (1.20 + 0.80) C_A] d\tau = dC_A$$

Integrating the above, we get the space-time of the PFR as follows:

$$\tau = \int d\tau = \int_{C_{A0}=2}^{C_{Af}} \frac{1}{3 - 2C_A} dC_A = \left[\frac{\ln(3 - 2C_A)}{-2} \right]_2^{C_{Af}}$$

which gives

$$-2\tau = \ln(2C_{Af} - 3)$$

and therefore, C_{Af} can be written as follows:

$$C_{Af} = \frac{3 + e^{-2\tau}}{2} \quad (6.80)$$

From the definition of x_A , we can relate x_{Af} to C_{Af} for a liquid-phase reaction as

$$x_{Af} = \frac{F_{A0} - F_{Af}}{F_{A0}} = \frac{F_{A0}/v - F_{Af}/v}{F_{A0}/v} = \frac{C_{A0} - C_{Af}}{C_{A0}}$$

which gives

$$C_{Af} = C_{A0} (1 - x_{Af}) = 2 (1 - x_{Af}) \quad (6.81)$$

Combining (6.80) and (6.81), we get

$$2(1 - x_{Af}) = \frac{3 + e^{-2\tau}}{2}$$

which is reduced to the following expression required by the problem statement:

$$x_{Af} = 1 - \frac{3 + e^{-2\tau}}{4} = 0.25[1 - e^{-2\tau}] \quad (6.82)$$

Plot of the x_{Af} versus τ is attached as Set6FigQ10, which shows that x_{Af} reaches 0.25 as τ approaches large values.

b) To determine the equilibrium conversion of A , let us start with the fact the overall reaction rate of A takes zero value at equilibrium since the forward reaction rate equal the backward reaction rate at equilibrium. Equating (6.75) and (6.76), therefore, gives

$$k_f C_A = k_b C_B \quad \text{at equilibrium.}$$

Using (6.79) in the above we get

$$k_f C_A = k_b (C_{A0} + C_{B0} - C_A) \quad \text{at equilibrium.}$$

which reduces to

$$C_{A,eqm} = \frac{k_b (C_{A0} + C_{B0})}{k_f + k_b} = \frac{1.20 \times (2.00 + 0.50)}{1.20 + 0.80} = 1.5 \text{ mol/m}^3.$$

where $C_{A,eqm}$ is the equilibrium concentration of A .

Using (6.81), the equilibrium conversion of A could be determined as follows:

$$x_{A,eqm} = \frac{1 - C_{A,eqm}}{2} = \frac{1 - 1.5}{2} = 0.25 = 25\%$$

The plot of the x_{Af} versus τ , attached as Set6FigQ10, also showed that x_{Af} reaches an equilibrium value of 0.25.

Space-time required to achieve 95% of the equilibrium conversion of A in the exit stream of the PFR can be calculated using (6.82) as follows:

$$0.95 \times 0.25 = 0.25[1 - e^{-2\tau}]$$

which gives

$$\tau = \frac{\ln(1 - 0.95)}{-2} = 1.4979 \approx 1.5 \text{ min.}$$

Note:

Solutions to Q11 and Q12 are not provided since they are part of Assignment 2.
