Problem-1: Presently 90% of reactant A is converted into product by a second order reaction in a single mixed flow reactor. We propose to place a second reactor similar to the one being used in series with it.

- (i) For the same treatment rate as that used presently, how will this addition of reactor affect the conversion of reactant?
- (ii) For the same 90% conversion, by how much can the treatment rate be increased in the latter case?

Solution: Consider the case of a single mixed flow reactor/CSTR.

For CSTR, we have

$$\frac{\tau}{C_{Ao}} = \frac{X_A}{(-r_A)}$$

For second order reaction:

$$(-r_A) = k C_A^2 = k C_{Ao}^2 (1 - X_A)^2 \text{ for } \epsilon_A = 0$$

$$\frac{\tau}{C_{Ao}} = \frac{X_A}{k C_{Ao}^2 (1 - X_A)^2}$$

$$\tau k C_{Ao} = \frac{X_A}{(1 - X_A)^2}$$
We have,
$$X_A = 0.90$$

$$\tau k C_{Ao} = \frac{0.90}{(1 - 0.90)^2}$$

$$\tau k C_{Ao} = 90$$

(i) Now, we will find the conversion that can be achieved using two equal-size CSTRs in series.

For CSTR-2 in series with the first one:

$$\frac{\tau_2}{C_o} = \frac{X_2 - X_1}{(-r)_2}$$

 $(-r)_2$ is evaluated at X_2

$$(-r)_2 = k C_0^2 (1 - X_2)^2 = k C_2^2$$

$$\frac{\tau_2}{C_0} = \frac{X_2 - X_1}{k C_0^2 (1 - X_2)^2}$$

$$\tau_2 k C_0 = \frac{X_2 - X_1}{(1 - X_2)^2}$$

For CSTR-1, we have

$$\tau_1 k C_0 = \frac{X_1}{(1 - X_1)^2} = 90, \quad X_1 = 0.90$$

$$\tau_1 = 90/k C_0$$

In two CSTRs in series $X_1 = 0.90$ is the intermediate conversion (i.e. conversion leaving CSTR-1) and X_2 is the overall conversion from the system as a whole.

For equal-size CSTRs in series,

$$\begin{array}{rcl} \tau_1 = \tau_2 &=& \tau \\ \tau_2 = \tau_1 &=& 90/k \; C_o & \text{as } \tau_k C_{Ao} = 90 \\ \tau_2 \; k \; C_o &=& \frac{X_2 - X_1}{(1 - X_2)^2} \\ \left(\frac{90}{k \; C_o}\right) k \; C_o &=& \frac{X_2 - X_1}{(1 - X_2)^2} \\ 90 \; = & \frac{X_2 - 0.90}{(1 - X_2)^2} \\ 90 \; (1 - X_2)^2 &=& X_2 - 0.90 \\ 90 \; X_2^2 - 181 \; X_2 + 90.90 &=& 0 \\ \therefore & X_2 &=& 0.972 \; \dots \text{ (positive root)} \end{array}$$

So using two equal-size CSTRs in series, 97.2% conversion of A is achieved.

% increase in conversion =
$$\left(\frac{0.972 - 0.90}{0.90}\right) \times 100 = 8$$

So addition of second mixed flow reactor/CSTR of equal size in series with the first one results in 8% increase in the conversion.

Ans.

(ii) Now, we will consider the case of two equal-size CSTRs in series for obtaining 90% overall conversion.

$$\therefore X_2 = 0.90$$

For CSTR-1:

$$\frac{\tau_1}{C_0} = \frac{X_1}{(-r)_1}$$

$$(-r)_1 = k C_0 (1 - X_1)^2$$

$$\tau_1 = \frac{X_1}{k C_0 (1 - X_1)^2}$$

Similarly, for CSTR-2:

$$\frac{\tau_2}{C_o} = \frac{X_2 - X_1}{(-r)_2}$$

$$(-r)_2 = k C_o (1 - X_2)^2$$

$$\tau_2 = \frac{X_2 - X_1}{k C_o (1 - X_2)^2}$$

For equal-size CSTRs in series,

$$\tau_1 = \tau_2 \quad (= \tau)$$

$$\frac{X_1}{k C_0 (1 - X_1)^2} = \frac{X_2 - X_1}{k C_0 (1 - X_2)^2}$$

$$\frac{X_1}{(1 - X_1)^2} = \frac{X_2 - X_1}{(1 - X_2)^2}$$

$$X_2 = 0.90$$

$$\frac{X_1}{(1 - X_1)^2} = \frac{0.90 - X_1}{(1 - 0.90)^2}$$

$$X_1 = (90 - 100 X_1) (1 - X_1)^2$$

Solving by trial and error method, For $X_1 = 0.75$, 0.76, 0.765...... and found $X_1 = 0.7635$, L.H.S = R.H.S

$$\tau_{2} = \frac{X_{2} - X_{1}}{k C_{0} (1 - X_{2})^{2}}$$

$$\tau_{2} k C_{0} = \frac{0.90 - 0.7635}{(1 - 0.90)^{2}}$$

$$= 13.65$$

$$\tau_{1} = \frac{X_{1}}{k C_{0} (1 - X_{1})^{2}}$$

$$\tau_{1} k C_{0} = \frac{X_{1}}{(1 - X_{1})^{2}}$$

$$= \frac{0.7635}{(1 - 0.7635)^{2}}$$

$$= 13.65$$

$$\tau_{2} = \tau_{1} = 13.65/k C_{0}$$

$$\tau_{1} = \tau_{2} = \tau \text{ for}$$

$$\tau_{N \text{ reactors}} = N \tau_{i}$$

$$(\tau)_{N=2} = 2 \times 13.65/k C_{0} = 27.3/k C_{0}$$

Single CSTR with 90% conversion,

$$\tau k C_{o} = 90$$

$$(\tau)_{N=1} = 90/k C_{o}$$

$$\frac{(\tau)_{N=2}}{(\tau)_{N=1}} = \frac{(V/v)_{N=2}}{(V/v)_{N=1}}$$

$$V_{N=2} = 2 V_{N=1}$$

$$(v)_{N=2} = \frac{2 (V)_{N=1}}{(V)_{N=1}} \times \frac{(\tau)_{N=1}}{(\tau)_{N=2}} \times (v)_{N=1}$$

$$(v)_{N=2} = \frac{2 \times 90}{k C_{o}} \times \frac{1}{\left(\frac{27.3}{k C_{o}}\right)} \times (v)_{N=1}$$

$$(v)_{N=2} = \frac{2 \times 90}{27.3} \times (v)_{N=1}$$

$$= 6.59 (v)_{N=1}$$

$$\approx 6.6 (v)_{N=1}$$

So the treatment capacity will be increased by 6.6 times than that of the single reactor

- If we use parallel connection, $F_{A0} = F_{A01} + F_{A02}$ and $F_{A01} = F_{A01}$
- $F_{AO} = 2F_{AO1}$, so treatment rate will be doubled.

Problem -2 Substance A reacts according to second-order kinetics. 95% conversion of A is achieved in a single flow reactor. We buy a second reactor identical to the first. For the same 95% conversion, by how much is the capacity increased if we operate these two reactors in parallel or in series?

- (i) The reactors are both plug flow.
- (ii) The reactors are both mixed flow.

Solution: $A \rightarrow \text{products} \dots \text{second order reaction}.$

$$-r_A = k C_A^2$$
 and $X_A = 0.95$

$$\frac{V}{F_{Ao}} = C_{Ao} \int_{0}^{X_A} \frac{dX}{(-r_A)}$$
 ... performance equation for PFR.

(i) For the two identical PFRs in series,

$$\frac{V_1}{F_o} = C_o \int_0^{X_1} \frac{dX}{(-r)}, \frac{V_2}{F_o} = C_o \int_{X_1}^{X_2} \frac{dX}{-r}$$

$$\frac{V_1 + V_2}{F_o} = C_o \int_0^{X_1} \frac{dX}{(-r)} + C_o \int_{X_1}^{X_2} \frac{dX}{-r} = C_o \int_0^{X_2} \frac{dX}{(-r)}$$

$$V_1 = V_2 = V$$

$$\frac{2V}{F_o} = C_o \int_0^{X_2} \frac{dX}{(-r)} = C_o \int_0^{0.95} \frac{dX}{(-r)}$$

For one (single) PFR,
$$\frac{V}{F_{Ao}} = C_o \int_{0.95}^{0.95} \frac{dX}{(-r_A)}$$

RHS of equations (1) and (2) remain the same (unchanged for one PFR as well as for two identical PFRs in series).

$$2V/F_o = V/F_{Ao}$$

 $F_o = 2 F_{Ao}$

:. Feed rate can be doubled.

... Ans.

For plug flow reactors in parallel, τ should be identical for the conversion to be the same in each parallel reactor (parallel line).

$$\tau_1 = \tau_2$$

For identical reactors:

$$V_1 = V_2$$

we have,

$$F_o = (F_o)_1 + (F_o)_2$$

For reactors in parallel:

$$V/(F_o)_1 = V/(F_o)_2$$

 $(F_o)_1 = (F_o)_2$

$$F_o = 2(F_o)_1$$

So the feed rate can be doubled.

Ans.

(ii) For a single CSTR/mixed flow reactor:

$$\tau = \frac{C_{Ao} V}{F_{Ao}} = \frac{C_{Ao} X_A}{(-r_A)}$$

$$\begin{array}{lll} \tau\,k\,\,C_{Ao} &=& 380 \\ \tau_{N=1} &=& 380/k\,\,C_o & (as\,C_o = C_{Ao}) \\ \\ (v)_{N=2} &=& \frac{(V)_{N=2}}{(V)_{N=1}} \times \frac{\tau_{N=1}}{\tau_{N=2}} \times (v)_{N=1} \\ \\ (V)_{N=2} &=& 2\,\,(V)_{N=1} \\ \\ (v)_{N=2} &=& \frac{2\,\,(V)_{N=1}}{(V)_{N=1}} \times \frac{380/k\,\,C_o}{78.4/k\,\,C_o} \times (v)_{N=1} \\ \\ (v)_{N=2} &=& 9.694\,\,(v)_{N=1} \\ &=& 9.7\,\,(v)_{N=1} \\ \\ (F_{Ao})_{N=2} &=& 9.7\,\,(F_{Ao})_{N=1} \\ \end{array}$$

Therefore, two identical CSTRs in series to achieve the overall conversion 95% the feed rate is 9.7 times of the feed rate of single CSTR.