P- 5.9

Liquid phase reaction

~~A → B~~ $A + B \rightarrow C$

- elementary kinetics
- isothermal

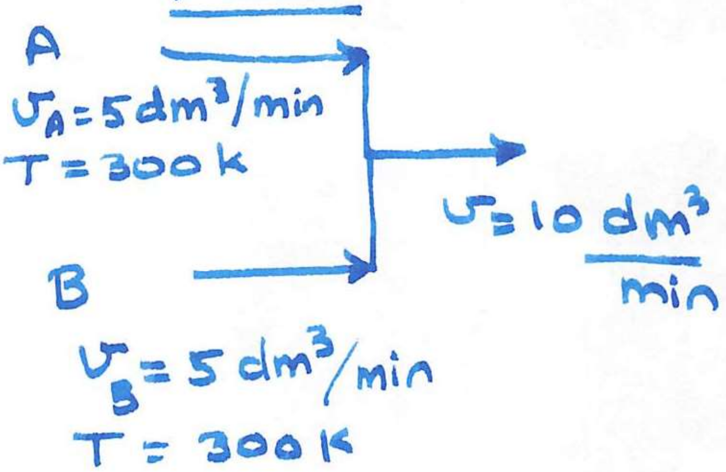
$C_A, C_B = 2\ M$

$k = 0.07\ \frac{dm^3}{mol \cdot min}$

$E = 20\ \frac{kcal}{mol}$

$R = 1.987\ \frac{cal}{mol\ K}$

Feed:



Reactors

CSTR:

$V = 200\ dm^3$

$T = 77°C$ or

$T = 0°C$

PFR

$V = 800\ dm^3$

A.) CSTR @ 77°C Vs PFR

$T = 350\ K$

$$k = 0.07\ \exp \frac{20000}{1.987}\left[\frac{1}{300} - \frac{1}{350}\right]$$

$k = 8.45\ dm^3/mol \cdot min$

CSTR

~~$X = V d$~~

$$X = \frac{V(-r_A)}{F_{A0}}$$

$F_{A0} = 2 \times 5$
$= 10 \ \frac{mol}{min}$

$-r_A = k C_A C_B$
$= k\, C_{A0}(1-X)\, C_{B0}(1-X)$

$C_{A0} = C_{B0}$

$\therefore -r_A = k\, C_{A0}^2 (1-X)^2$

$$X = \frac{V\left(C_{A0}^2 (1-X)^2\right)}{F_{A0}}$$

$$X = \frac{200 \times 8.45 \times 1 \times (1-X)^2}{10}$$

$X = 0.925$

PFR

$V = 800 \ dm^3$
$T = 300 \ K$

$$F_{A0} \frac{dX}{dV} = -r_A$$

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}} = \frac{k C_{A0}^2 (1-X)^2}{F_{A0}}$$

$$dx = \frac{0.07 \cdot 1^2 (1-x)^2}{10} dV$$

$$\frac{x}{1-x} = 0.007V$$

$\Rightarrow x = 0.85$

→ **Use CSTR**

b) Batch reactor

$V = 200\ dm^3$

$N_{A0}, N_{B0} = 200$ moles

$x = 0.9$

Assume isothermal

~~$t = \int r_A$~~ $t = N_{A0} \int_0^x \frac{dx}{-r_A V}$

$$t = \frac{200}{8.45 \times 1^2 \times 200} \int_0^x \frac{dx}{(1-x)^2}$$

$t = 1.06$ min

c) $T = 273\ K$

$$\ln \frac{k_2}{k_1} = \frac{E}{R}\left[\frac{1}{T_1} - \frac{1}{T_2}\right]$$

$k_1 = 0.07\ \frac{dm^3}{mol \cdot min}$ $T_2 = 273\ K$

$T_1 = 300\ K$

$E = 20\ kcal$

$\Rightarrow k = 2.54 \times 10^{-3}$

$$\Rightarrow t = \frac{200 \times 9}{2.54 \times 10^{-3} \times 200} = 3543\ min$$

$t = 2.5$ days.

d) CSTR/ PFR connected in series

$$x_{CSTR} = \frac{V \cdot -r_A|exit}{F_{A0}}$$

$$x = \frac{200 \times 0.07 \times 1^2 \times (1-x)^2}{10}$$

$\Rightarrow x_{CSTR} = 0.44$

For PFR

$$F_{A0} \frac{dX}{dV} = -r_A$$

$$dX = \frac{~~0.07~~ \, k C_{A0}^2 (1-X)^2}{F_{A0}} dV$$

$$\int_{0.44}^{X} \frac{dX}{(1-X)^2} = \frac{0.07 \times 1^2 \times 800}{10}$$

$$\Rightarrow X = 0.736$$

CSTR and PFR connected in parallel

$$X_{CSTR} = \frac{200 \times 0.07 \times 1^2 \times (1-X)^2}{5}$$

$$X_{CSTR} = 0.56$$

$X_{PFR} \Rightarrow$

$$\int_{0}^{X} \frac{dX}{(1-X)^2} = \frac{0.07 \times 1^2 \times 800^2}{5}$$

$$= 0.92$$

$$X_{Final} = \frac{0.56 + 0.92}{2} = 0.74$$

e) To process same amount of species -

batch reactor must handle

$$2M \cdot 5\,\frac{dm^3}{min} \cdot 60\,\frac{min}{hr} \cdot 24\,\frac{hr}{day} = 14400\,\frac{mol}{day}$$

$$V = 14400 \cdot \frac{1\,dm^3}{day} = 14400\,\frac{dm^3}{day}$$

Time required for $x = 0.9$

$$\frac{dX}{dt} = \frac{-r_A V}{N_{A0}} = \frac{k C_{A0}^2 (1-X)^2 V}{N_{A0}}$$

$$t_R = \frac{N_{A0}}{V k C_{A0}^2} \frac{X}{1-X} \qquad \frac{N_{A0}}{V} = C_{A0}$$

$$t_R = \frac{1}{k C_{A0}} \frac{X}{1-X} \Rightarrow \frac{1}{4.2 \times 1\,\frac{dm^3}{mol \cdot hr}} \times \frac{0.9}{0.1}$$

$$t_R = 2.14\ hr$$

Assuming it takes 3 hours to fill, empty, and heat to rxn temperature

$t_f = 3$ hr

$t_T = t_R + t_f$

$t_T = 2.14 + 3$ hr $= 5.14$ hr

$\therefore$ we can run 4 batches in a day

$$V = \frac{14400}{4} = 3600 \text{ dm}^3$$