Q. 1.5

Assumptions

a) Batch reactor
- → No input / output
- completely mixed

b) CSTR
- → ~~N~~ Steady state
- completely mixed

c) PFR
- steady state
- plug flow profile (No radial variation)
  - └ only axial variation of conc. and reaction rate

d) PBR
- Steady state
- No radial variation in properties of system

e) for reaction $A \longrightarrow B$

$-r_A$: number of moles of A reacting per unit time per unit volume ($mol/dm^3\ s$)

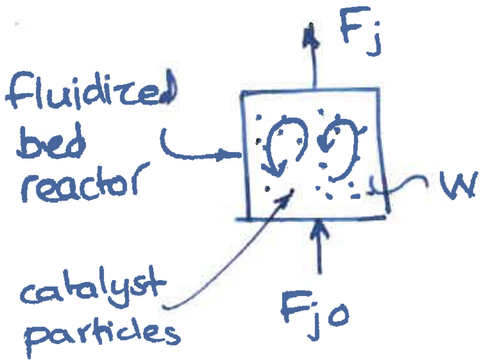
$-r_A'$: number of moles of A reacting per unit mass of catalyst per unit time ($mol/kg\ cat\ s$)

$-r_A$ is an intensive property

- it is a function of conc., temp, pressure, cat type etc.
- It is defined at any point within the system
- It is independent of amount

On the other hand extensive property is obtained by summing up the properties of individual subsystems within the total system; in this sense, $-r_A$ is independent of the extent of the system.

Q. 1.6 mole balance for fluidized bed reactor



rate of homogeneous reaction r_A :

Moles of A formed per unit volume of reactor per unit time

For catalytic reactions :

$-r'_A$: g mol of A reacted per g catalyst per s

$\Rightarrow$ mass of catalyst is the basis and not reactor volume

General mole balance :

$$F_{jo} - F_j + \int r_j \, dV = \frac{dN_j}{dt}$$

Assumptions : ~~4A~~
- steady state
- completely mixed

$$r_j = \rho_b \, r'_j$$

ρ_b : bulk density

$$\frac{\text{mol}}{\text{m}^3 \ \text{s}} \qquad \frac{\cancel{\text{kg}}}{\text{m}^3} \qquad \frac{\text{mol}}{\cancel{\text{kg}} \ \text{s}}$$

$$W = \rho_b V$$

weight of catalyst

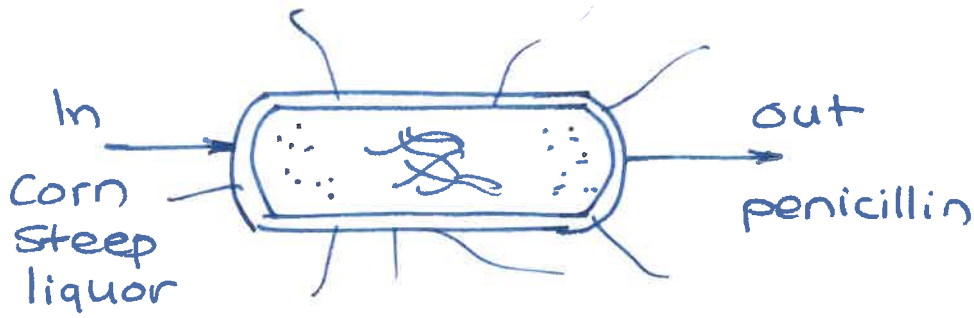
$$F_{j0} - F_j + \int \rho_b r_j \, dV = 0$$

$$\rho_b \, dV = dW$$

$$\therefore \quad F_{j0} - F_j + \int r_j' \, dW = 0$$

$$\Rightarrow \quad \boxed{W = \frac{F_{j0} - F_j}{r_j'}}$$

Q. 1.9 cell reactor



Assumptions

- well mixed
- RNA remains inside the cell
- ~~Steady state~~

a) Unsteady mass balance on

Corn steep liquor

$$F_{C0} - \cancel{F_C}^{\,0} + \int^V -r_C \, dV = \frac{dN_C}{dt}$$

$$F_{C0} + \int^V r_C \, dV = \frac{dN_C}{dt}$$

penicillin

$$\cancel{F_{P0}}^{\,0} - F_P + \int^V r_P \, dV = \frac{dN_P}{dt}$$

$$\int^V r_P \, dV - F_P = \frac{dN_P}{dt}$$

RNA

$$\cancel{F_{R0}}^{\,0} - \cancel{F_R}^{\,0} + \int^V r_R \, dV = \frac{dN_R}{dt}$$

$$\int^V r_R \, dV = \frac{dN_R}{dt}$$

In cell's stationary state
→ steady state applies.

Balance equations:

∴ for corn steep liquor

$$V = \frac{F c_o}{r_c}$$

for penicillin

$$V = \frac{F p}{r_p}$$

<u>for RNA</u>: No generation / ~~consumption~~ destruction

1·4 d

Assuming that the volumetric flow rates entering and leaving the basin are identical

$$\upsilon = \upsilon_0$$

Show that the unsteady mass balance on CO within the basin becomes

$$F_{CO,A} + F_{CO,S} - \upsilon_0 C_{CO} = V \cancel{\frac{dC_{O}}{dt}} \frac{dC_{CO}}{dt}$$

$\Rightarrow$ General mole balance

in - out + generation - consumption

= accumulation

~~Input~~ In : $F_{CO,A} + F_{CO,S}$

out : $\upsilon_0 C_{CO}$

generation = 0

consumption = 0

$$\text{accumulation} = \frac{dN_{CO}}{dt}$$

$$= \frac{dVC_{CO}}{dt} = V\frac{dC_{CO}}{dt}$$

$$\therefore F_{CO,A} + F_{CO,S} - \upsilon_0 C_{CO} = V\frac{dC_{CO}}{dt} \quad (1)$$

1·4 e Verify the solution to previous equation is

$$t = \frac{V}{\upsilon_0}\ln\left(\frac{[F_{CO,A} + F_{CO,S}] - \upsilon_0 C_{CO,0}}{[F_{CO,A} + F_{CO,S}] - \upsilon_0 C_{CO,f}}\right)$$

$\Rightarrow$ Rearranging (1)

$$dt = \frac{V\,dC_{CO}}{F_{CO,A} + F_{CO,S} - \upsilon_0 C_{CO}}$$

$$\Rightarrow \frac{dt}{V} = \frac{dC_{CO}}{(F_{CO,A} + F_{CO,S}) - \upsilon_0 C_{CO}}$$

Let $(F_{CO,A} + F_{CO,S}) = a$

$-\upsilon_0 = b$

$$\therefore \frac{dt}{V} = \frac{dC_{CO}}{a + b\,C_{CO}}$$

$$\therefore \int_0^t \frac{dt}{V} = \int_{C_{CO,0}}^{C_{CO,F}} \frac{dC_{CO}}{a + b\,C_{CO}}$$

$$\int \frac{dx}{a+bx} = \frac{\cancel{\log}\ \ln(a+bx)}{b}$$

$$\therefore \frac{t}{V} = \frac{1}{-\upsilon_0} \ln\left[\frac{(F_{CO,A} + F_{CO,S}) - \upsilon_0 C_{CO,F}}{(F_{CO,A} + F_{CO,S}) - \upsilon_0 C_{CO,0}}\right]$$

$$\therefore t = \frac{V}{\upsilon_0} \ln\left[\frac{(F_{CO,A} + F_{CO,S}) - \upsilon_0 C_{CO,0}}{(F_{CO,A} + F_{CO,S}) - \upsilon_0 C_{CO,F}}\right]$$

P1-5 reaction $A \longrightarrow B$

- isothermal
- continuous flow reactor

$$v_0 = 10 \ dm^3/h$$

$$C_{A0} = 0.5 \ mol/dm^3$$

Calculate volume of CSTR and PFR required for 99 % conversion

$$C_A = 0.01 \, C_{A0}$$

a) $-r_A = k$ $\quad k = 0.05 \ \dfrac{mol}{h \ dm^3}$

CSTR : $V = \dfrac{F_{A0} - F_A}{-r_A}$

$$F_{A0} = C_{A0} v$$

$$F_A = C_A v = 0.01 \, C_{A0} v$$

$$\therefore \ V = \frac{v \left(C_{A0} - 0.01 \, C_{A0} \right)}{k}$$

$$= \frac{0.99 \times 10 \times 0.5}{0.05}$$

$$V = 99 \ dm^3$$

PFR

$$\frac{dF_A}{dV} = \cancel{-}\, r_A$$

$$F_A = C_A \upsilon_o \quad ; \quad F_{A0} = C_{A0} \upsilon_o$$

$$r_A = k$$

$$\cancel{V = \int}$$

$$\frac{d\, C_A \upsilon_o}{dV} = k$$

$$\frac{\upsilon_o}{k} \int_{C_{A0}}^{C_A} d\, C_A = \int_0^V dV$$

$$V = \frac{\upsilon_o}{k} (C_{A0} - C_A)$$

$$= \frac{10 \times 0.5\, (1 - 0.01)}{0.05}$$

$$V = 99 \text{ dm}^3$$

b) $-r_A = kC_A$

$k = 0.0001\ s^{-1}$

$= 0.0001\ \frac{1}{s} \cdot 3600\ \frac{s}{h}$

$k = 0.36\ h^{-1}$

<u>CSTR</u>: $V = \dfrac{F_{A0} - F_A}{-r_A}$

$F_{A0} = C_{A0} \cdot v$

$F_A = C_A \cdot v = 0.01\, C_{A0} v$

$-r_A = kC_A = 0.01\, C_{A0} k$

$$V = \frac{v(\cancel{C_{A0}} - 0.01\cancel{C_{A0}})}{k\, 0.01\, \cancel{C_{A0}}}$$

$$= \frac{10 \times 0.99}{0.36 \times 0.01} = 2750\ dm^3$$

<u>PFR</u>

$$\frac{dC_A v_0}{dV} = r_A = kC_A$$

$$\therefore \frac{v_0}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = \int_0^V dV$$

$$\frac{v_0}{k} \ln \frac{C_{A0}}{C_A} = V$$

$$V = \frac{10}{0.36} \ln\left(\frac{1}{0.01}\right)$$

$$V = 127.9 \ dm^3$$

c) $-r_A = k C_A^2$

$$k = 300 \ \frac{dm^3}{mol\ h}$$

CSTR

$$V = \frac{F_{A0} - F_A}{-r_A}$$

$$-r_A = k C_A^2 = 0.01^2 C_{A0}^2 k$$

$$V = \frac{\upsilon (C_{A0} - 0.01 C_{A0})}{300 \times (0.01\ C_{A0})^2}$$

$$= \frac{10\ (0.99)}{300 \times (0.01)^2 \times 0.5}$$

$$V = 660 \qquad dm^3$$

PFR

$$\frac{dC_A \upsilon_0}{dV} = r_A = k C_A^2$$

$$\Rightarrow \frac{\upsilon_0}{k} \int_{C_{A0}}^{C_A} \frac{dC_A}{C_A^2} = \int_0^V dV$$

$$\frac{\upsilon_0}{k}\left(\frac{1}{C_A} - \frac{1}{C_{A0}}\right) = V$$

$$V = \frac{v_0}{k\, C_{A0}} \left(\frac{1}{0.01} - 1 \right)$$

$$= \frac{10}{300 \times 0.5} \times 99$$

$$V = 6.6 \quad dm^3$$

d) Batch reactor

$C_A = 0.001\, C_{A0} \Rightarrow 99.9\%$ consumption

$V = 1000\ dm^3$

$C_{A0} = 0.5 \ \frac{mol}{dm^3}$

$$t = \int_{N_A}^{N_{A0}} \frac{dN}{-r_A V}$$

constant volume : $V = V_0$

$$t = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A}$$

zero order

$$t = \frac{1}{k}\left[C_{A0} - C_A\right]$$

$$= \frac{1}{k}\left[C_{A0} - 0.001\, C_A\right] = \frac{0.999\, C_{A0}}{k}$$

6

$$t = \frac{0.999 \times 0.5}{0.05}$$

$$\underline{t = 9.99\ h}$$

First order

$$t = \frac{1}{k}\ln\left(\frac{C_{A0}}{C_A}\right)$$

$$= \frac{1}{0.36}\ln\left(\frac{1}{0.001}\right)$$

$$\underline{t = 19.18\ h}$$

Second order

$$t = \frac{1}{k}\left[\frac{1}{C_A} - \frac{1}{C_{A0}}\right]$$

$$= \frac{1}{0.03}\left[\frac{1}{0.001} - \frac{1}{1}\right]\cdot\frac{1}{0.5}$$

$$= \frac{999}{0.03 \times 0.5}$$

$$\underline{t = 66600\ h}$$

P 1.8

$$2A \xrightarrow{k_1} B$$

$$-r_A = k_1 C_A^2$$

$$k_1 = 0.03 \ dm^3/mol\ s$$

$$C_{A_0} = 2 \ mol/dm^3$$

$$\upsilon_0 = 3 \ dm^3/s$$

$$C_A = 0.1 \ mol/dm^3$$

$\upsilon = \upsilon_0 \Rightarrow$ steady state

mole balance :

$$V = \frac{F_{A_0} - F_A}{-r_A}$$

$$-r_A = k C_A^2$$

$$V = \frac{F_{A_0} - F_A}{k C_A^2}$$

$$F_{A_0} = C_{A_0} \upsilon_0 = 2 \frac{ol}{m^3} \cdot 3 \frac{dm^3}{s} = 6 \frac{mol}{s}$$

$$F_A = C_A \upsilon \quad .1 \frac{mol}{dm^3} \cdot 3 \frac{dm^3}{s} = 0.3 \frac{mol}{s}$$

$$V = \frac{(6 - 0.3)}{0.03 \times 0.1^2}$$

$$V = \boxed{19000} \ dm^3$$