march 6 lecture → examples

• review steady-state condition for CFSTR:

mass balance:

$$\begin{pmatrix}\text{rate of}\\ \text{mass accum}\end{pmatrix} = \begin{pmatrix}\text{mass}\\ \text{flux in}\end{pmatrix} - \begin{pmatrix}\text{mass}\\ \text{flux out}\end{pmatrix} \pm \begin{pmatrix}\text{source/}\\ \text{sink}\end{pmatrix}$$

$$\frac{dC}{dt}\forall = QC_o - QC \underbrace{- kC\forall}_{\text{sink, first order}}$$

@ S.S. $\frac{dC}{dt} = 0$

$$0 = QC_o - QC - kC\forall$$

$$0 = \frac{Q}{\forall}C_o - \frac{Q}{\forall}C - kC$$

$$0 = \frac{C_o}{t_o} - \frac{C}{t_o} - kC$$

, note that $\frac{\forall}{Q} = t_o = \theta_H$ is hydraulic residence time (pg 6-14)

$$0 = \frac{C_o}{t_o} - \frac{C(1+kt_o)}{t_o}$$

$$\therefore \quad C = \frac{C_o}{1+kt_o}$$

- example, cascade of reactors (pg 6-26)

p- denotes products
$C_{pi} = 30\ g/m^3$, influent conc.
$r_p = -kC_p$, first order decay
$k = 0.2 d^{-1}$
$Q = 5 m^3/s$

$V_1 = 8.64 \times 10^5\ m^3$
$V_2 = 25.92 \times 10^5\ m^3$
$V_3 = 17.28 \times 10^5\ m^3$
$V_4 = 8.64 \times 10^5\ m^3$
$V_5 = 25.92 \times 10^5\ m^3$

- solution

step 1
- assume system is at steady-state (i.e $dC/dt = 0$)
- write mass balance equation for each reactor

① $0 = QC_{pi} - QC_{p1} - kC_{p1}V_1$

② $0 = QC_{p1} - QC_{p2} - kC_{p2}V_2$

③ $0 = QC_{p2} - QC_{p3} - kC_{p3}V_3$

④ $0 = QC_{p3} - QC_{p4} - kC_{p4}V_4$

⑤ $0 = QC_{p4} - QC_{p5} - kC_{p5}V_5$

step 2
- rearrange equations

from ① $C_{p1} = \frac{C_{pi}}{(1 + k\theta_{H1})}$

from ② $C_{p2} = \frac{C_{pi}}{(1+k\theta_{H1})(1+k\theta_{H2})}$

from ③ $C_{p3} = \frac{C_{pi}}{(1+k\theta_{H1})(1+k\theta_{H2})(1+k\theta_{H3})}$

from ④ $C_{p4} = \frac{C_{pi}}{(1+k\theta_{H1})(1+k\theta_{H2})(1+k\theta_{H3})(1+k\theta_{H4})}$

from ⑤ $C_{p5} = \frac{C_{pi}}{(1+k\theta_{H1})(1+k\theta_{H2})(1+k\theta_{H3})(1+k\theta_{H4})(1+k\theta_{5})}$

- aside to step 2

① $0 = QC_{pi} - QC_{p1} - kC_{p1}\forall_1 \rightarrow C_{p1} = \frac{C_{pi}}{(1+k\theta_{H1})}$

② $0 = QC_{p1} - QC_{p2} - kC_{p2}\forall_2 \rightarrow C_{p2} = \frac{C_{p1}}{(1+k\theta_{H2})}$

- sub in C_{p1}

$$C_{p2} = \frac{C_{pi}}{(1+k\theta_{H1})(1+k\theta_{H2})}$$

- similarily, develop C_{p3} to C_{p5}

- note, if reactors are of equal volume

then $\theta_{H1} = \theta_{H2}$

giving $C_{p2} = \frac{C_{pi}}{(1+k\theta_H)^2}$

thus, for CFSTR-n $\quad C_n = \frac{C_o}{(1+k\theta_H)^n}$

step 3 • substitute values and solve

• calculate θ_{H_i}:

$$\theta_{H_1} = \frac{V_1}{Q} = \frac{(8.64 \times 10^5)}{(5)} = 172800 \text{ s} \rightarrow 2 \text{ day}$$

$$\theta_{H_2} = 518400 \text{ s} \rightarrow 6 \text{ d}$$

$$\theta_{H_3} = 345600 \text{ s} \rightarrow 4 \text{ d}$$

$$\theta_{H_4} = 172800 \text{ s} \rightarrow 2 \text{ d}$$

$$\theta_{H_5} = 518400 \text{ s} \rightarrow 6 \text{ d}$$

* note, θ_H and k require consistent units.

$$C_{p_1} = \frac{(30)}{(1 + (0.2)(2))} = 21.4 \text{ g/m}^3$$

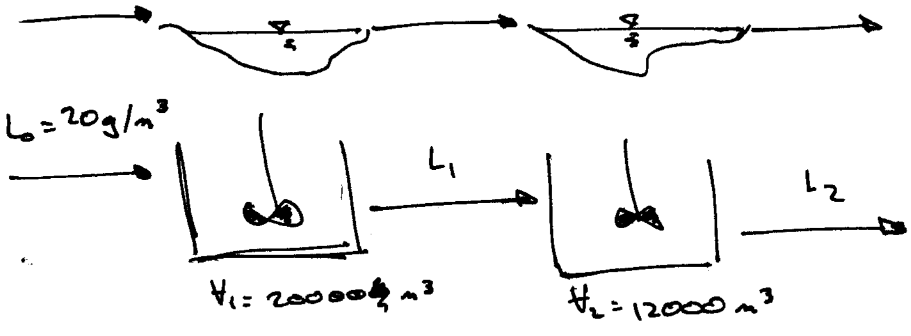
$$C_{p_2} = \frac{(30)}{(1 + (0.2)(2))(1 + (0.2)(6))} = 9.7 \text{ g/m}^3$$

$$C_{p_3} = 5.41 \text{ g/m}^3$$

$$C_{p_4} = 3.87 \text{ g/m}^3$$

$$C_{p_5} = 1.76 \text{ g/m}^3$$

- <u>example,</u> ass.3, q. 11



$Q = 4000 m^3/d$

$k = 0.35 d^{-1}$

- <u>solution</u>

- assume steady-state

$$L_1 = \frac{L_o}{(1 + k\theta_{H_1})}, \quad \theta_{H_1} = \frac{V_1}{Q} = \frac{(20000)}{(4000)} = 5d$$

$$L_1 = \frac{(20)}{(1 + (0.35)(5))}$$

$$L_1 = 7.27 \ g/m^3$$

$$L_2 = \frac{L_1}{(1 + k\theta_{H_2})}, \quad \theta_{H_2} = \frac{V_2}{Q} = \frac{(12000)}{(4000)} = 3d$$

$$L_2 = \frac{(7.27)}{(1 + (0.35)(3))}$$

$$L_2 = 3.55 \ g/m^3$$

- **example**, ass3, q10 - rxn rates

$$A \xrightarrow{k_1} B \qquad A \xrightarrow{k_2} C$$

$$A \xrightarrow{k_1} B$$

$$A \xrightarrow{k_2} C$$

- **solution**

  - for a single first order rxn

    $$\frac{\partial A}{\partial t} = -kA$$

A

  - for our situation, parallel first order rxns

    $$\frac{\partial A}{\partial t} = -k_1 A - k_2 A$$, neg. rxn rate b/c A is being consumed

    $$\frac{\partial A}{\partial t} = -(k_1 + k_2) A$$

integrate: $A = A_0 e^{-(k_1+k_2)t}$

aside, integration to determine A expression

$$\frac{\partial A}{\partial t} = -(k_1+k_2) A$$

$$\int \frac{1}{A} \partial A = -(k_1+k_2) \int \partial t$$

$$\ln A + C_1 = -(k_1+k_2) t + C_2$$

$$\ln A = -(k_1+k_2) t + (C_2 - C_1)$$

$$A = e^{-(k_1+k_2)t} \cdot e^{(c_2-c_1)} \quad , \quad A_0 = e^{(c_2-c_1)} = \text{const.}$$

$$A(t) = A_0 e^{-(k_1+k_2)t}$$

determine A_0, @ $t=0 \rightarrow [A]=1$ mol/L

$$(1) = A_0 e^{-(k_1+k_2)(0)}$$

$$A_0 = 1$$

$$\therefore \; A(t) = e^{-(k_1+k_2)t}$$

- sub in values & solve for k_1 & k_2

@ $t = 16$ min $\rightarrow [A] = 0.01$ mol/L

$$(0.01) = e^{-(k_1+k_2)(16)}$$

$$\ln(0.01) = -(k_1+k_2)(16)$$

$$k_1+k_2 = 0.287 \text{ min}^{-1}$$

B

- single first order rxn

$$\frac{dB}{dt} = k_1 A \quad , \text{ pos. rxn rate b/c B is being produced}$$

$$\frac{dB}{dt} = k_1 A_0 e^{-(k_1+k_2)t}$$

integrate:
$$B = \frac{-k_1}{k_1+k_2} A_0 e^{-(k_1+k_2)t} + D$$

D ← const. of integration

determine D, @ t=0 → [B] = 0 mol/L

$$(0) = \frac{-k_1}{k_1+k_2} A_0 e^{-(k_1+k_2)(0)} + D$$

$$D = \frac{k_1 A_0}{k_1+k_2}$$

$$\therefore B(t) = -\frac{k_1}{k_1+k_2} A_0 e^{-(k_1+k_2)t} + \frac{k_1 A_0}{k_1+k_2}$$

$$B(t) = \frac{-k_1}{k_1+k_2} A + \frac{k_1 A_0}{k_1+k_2}$$

$$B(t) = \frac{k_1}{k_1+k_2} (A_0 - A)$$

- sub in values to solve for k_1 & k_2

@ t = 16 min → [A] = 0.01 mol/L , [B] = 0.66 mol/L

$$(0.66) = \frac{k_1}{k_1+k_2} ((1) - (0.01))$$

$$\frac{k_1}{k_1+k_2} = 0.667$$

from A, we know $k_1 + k_2 = 0.287$

$$\therefore \frac{k_1}{(0.287)} = 0.667 \rightarrow k_1 = 0.191 \text{ min}^{-1}$$

$$k_2 = 0.287 - (0.191) \rightarrow k_2 = 0.096 \text{ min}^{-1}$$

C · single first order rxn

$$\frac{dC}{dt} = k_2 A$$, pos. rxn rate b/c C is being produced

$$\frac{dC}{dt} = k_2 A_o e^{-(k_1+k_2)t}$$

integrate: $C = \frac{-k_2}{k_1+k_2} A_o e^{-(k_1+k_2)t} + E$

determine E, assume @ t=0 → [C] = mol/L
i.e. b/f rxn has started there is no C product.

$$(0) = \frac{-k_2}{k_1+k_2} A_o e^{-(k_1+k_2)(0)} + E$$

$$E = \frac{k_2}{k_1+k_2} A_o$$

$$\therefore\ C(t) = \frac{-k_2}{k_1+k_2} A_o e^{-(k_1+k_2)t} + \frac{k_2}{k_1+k_2} A_o$$

$$C(t) = \frac{-k_2}{k_1+k_2} A + \frac{k_2}{k_1+k_2} A_o$$

$$C(t) = \frac{k_2}{k_1+k_2} (A - A_o)$$

- use C(t) to populate table

t (min)	[A] mol/L	[B] mol/L	[C] mol/L
0	1.00	0	0
2	0.55	0.30	0.15
4	0.30	0.47	0.23
8	0.09	0.61	0.30
16	0.01	0.66	0.33

e.g. $C(2) = \frac{(0.096)}{(0.287)}\left((1) - (0.55)\right)$

$C(2) = 0.15$ mol/L