$A + P \rightarrow P + P$

$r = -kC_A C_P$

$C_{A_0} = 0.99$ mol/L

$C_{P_0} = 0.01$ mol/L

$C_A = 0.10$ mol/L

$C_P = 0.9$ mol/L

$k = 1$ L/mol-min

1) what is τ_m (mfr)?

2) what is τ_p (pfr)?

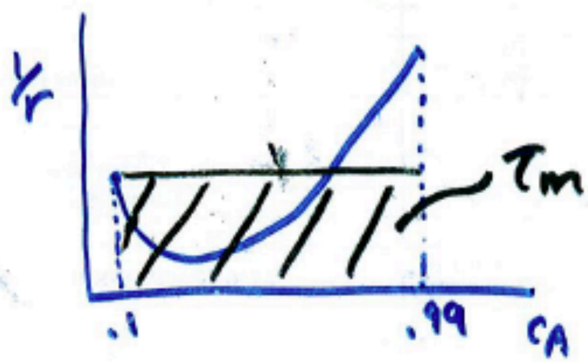
3) what is minimum size of pfr, mfr combo to achieve rxn?

1) Mixed flow reactor

$$\tau_m = \frac{C_{A_0} - C_A}{kC_A C_P}$$

$\Rightarrow$ mass balance $C_A + C_P = 1.0$

$$= \frac{C_{A_0} - C_A}{kC_A(1 - C_A)} = \frac{(.99) - (.10)}{(1)(.1)(1 - .1)} = \underline{\underline{9.89 \text{ min}}}$$



2) PFR

$$\tau_p = \int_{C_{A0}}^{C_A} \frac{dC_A}{r} = \int \frac{dC}{-kC_A(1-C_A)}$$

$C_T = C_A + C_P = 1$

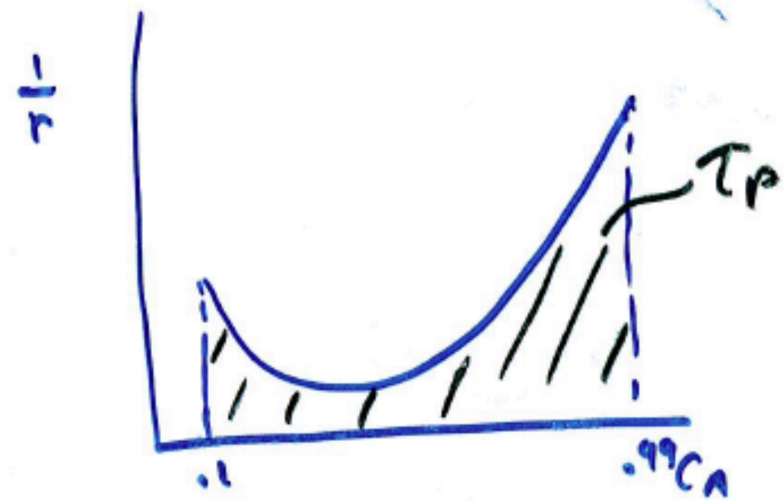
$$= \frac{-1}{kC_T}\left[\int \frac{dC}{C_A} + \int \frac{dC}{1-C_A}\right]$$

$$= \frac{1}{-kC_T}\left[\ln C_A/C_{A0} - \ln\frac{(1-C_A)}{(1-C_{A0})}\right]$$

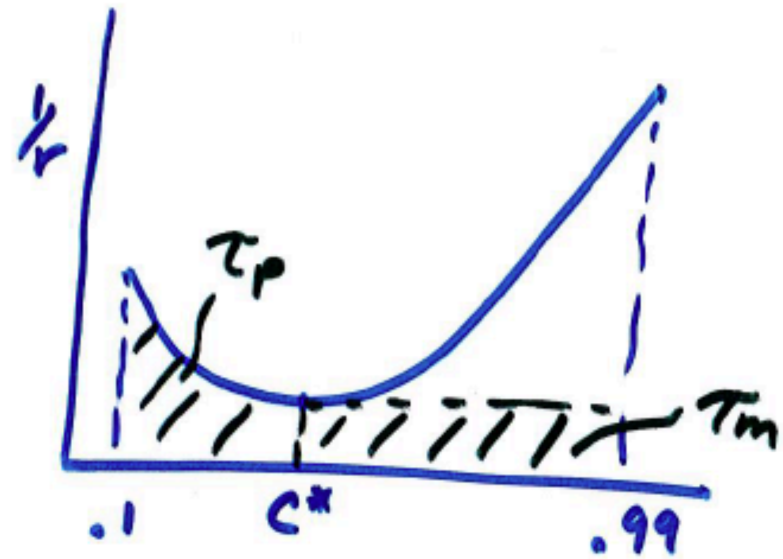
$$= \frac{1}{kC_T}\left[\ln\left(C_{A0}/C_A\right) + \ln\frac{(1-C_A)}{(1-C_{A0})}\right]$$

$$= \frac{1}{kC_T}\ln\frac{[C_{A0}/1-C_{A0}]}{[C_A/1-C_A]}$$

$$= \frac{1}{(1)(1)}\ln\frac{(.99/.01)}{(.1)/(.9)} = \underline{\underline{6.792\ \text{min}}}$$



3) Min. τ (combo, $\tau_m + \tau_p$)



must find C*

$$\frac{dr}{dC} = \frac{d}{dC}\left[-kC(1-C)\right] = 0$$

$$= k\,dC(1-C) + kC(-dC)$$

$$\Rightarrow 1-C = C \Rightarrow C = 0.5$$

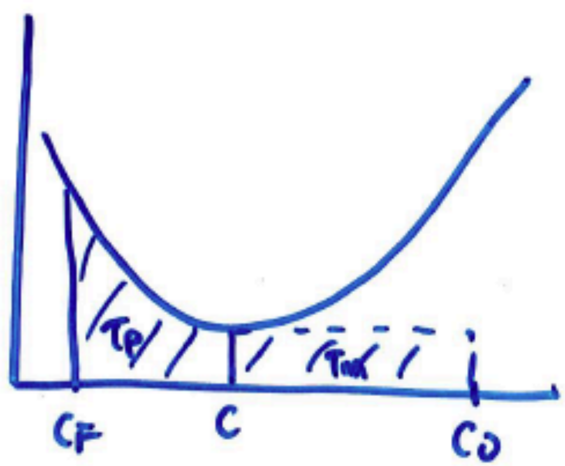
3) $$\tau_m = \frac{C_0 - C}{kC(1-C)} = \frac{(0.99-0.5)}{(1)(0.5)(1-0.5)} = 1.96 \text{ min}$$

$$\tau_p = \frac{1}{kC_T} \ln \frac{[C/(1-C)]}{[C_F/(1-C_F)]}$$

$$= \frac{1}{(1)(1)} \ln \frac{(0.5)/(1-0.5)}{(0.1/(1-0.1))}$$

$$= 2.20 \text{ min}$$

$$\tau_{total} = 1.96 + 2.20 = 4.16 \text{ min}$$

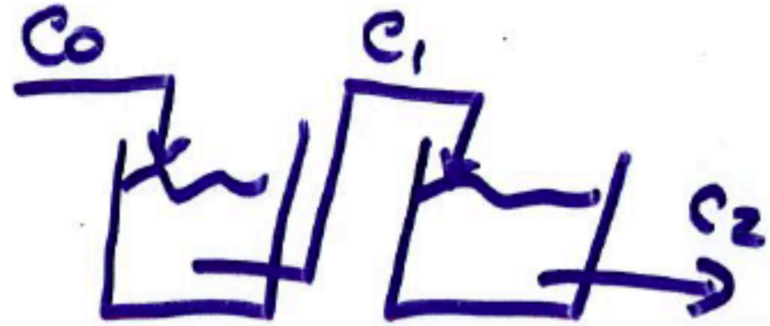


2 MFR in series,

$\tau = 5.3$

$k = 0.07 \frac{L}{mol\text{-}hr}$

$C_0 = 18$ mol/L



What is final conversion?

What are intermediate concentrations?

2nd order rxn

$$K\tau = \frac{C_0 - C}{C^2} \Rightarrow K\tau C^2 + C - C_0 = 0$$

$$C = \frac{-1 + \sqrt{1 + 4K\tau C_0}}{2K\tau}$$

$$C_1 = \frac{-1 + \sqrt{1 + 4(.07)(5.3)(18)}}{2(.07)(5.3)} = 5.747 \text{ mol/L}$$

$$C_2 = \frac{-1 + \sqrt{1 + 4 k \tau C_1}}{2 k \tau}$$

$$= \frac{-1 + \sqrt{1 + 4(.07)(5.3)(5.747)}}{2(.07)(5.3)}$$

$$= \underline{\underline{2.812}} \text{ mol/L}$$

$$X = \frac{C_0 - C_2}{C_0} = \underline{\underline{0.844}}$$

You are VP of technology for I Co.

You have a 500 L MFR (ideal) in which you can make either product B or Product C, from raw material A.

$$A \rightarrow 2B \quad \text{or} \quad 2A \rightarrow C$$

$$k = 0.3\ \text{min}^{-1} \qquad k = 0.2\ \text{min}^{-1}$$

Data: $C_{A0} = 0.5$ mol/L

$v = 50$ L/min

A costs \$5/mol

B sells for \$15/mol

C sells for \$40/mol

Which product would you make to maximize profits?

Soln

Profit = Sales - Expenses

$$\Downarrow \qquad\qquad \Downarrow$$

B or C $\qquad$ A

MUST CALC. USAGE RATE OF A

& production rates of B/C

& multiply by \$/mol

1) How much A is used?

$$v C_{A_0} = \frac{50\,L}{min}\left|\frac{0.5\,mol}{L}\right. = 25\,\frac{mol}{min}$$

2) How much B or C produced?

$$\tau = \frac{V}{v} = \frac{500}{50} = 10\text{ min}$$

Both 1st order rxn's

$$C_A = \frac{C_{A0}}{1 + \tau k}$$

B

$$C_A = \frac{0.5}{1+(10)(.3)}$$

$$= 0.125 \text{ mol/L}$$

$$\therefore X_A = \frac{0.5-0.125}{0.5}$$

$$= 0.75$$

$\therefore$ Produces

$$\frac{25 \text{ mol}}{\text{min}} \Big| \, 0.75 \, \Big| \, 2$$

$$= 37.5 \text{ mol/min } B$$

Sales: $(37.5)(15) = \$562.50$

Expenses: $(25)(5) = \$125.00$

Profit ($/min) $437.50

C

$$C_A = \frac{0.5}{1+(10)(.2)}$$

$$= 0.166667$$

$$\therefore X_A = \frac{0.5-.16667}{0.5}$$

$$= 0.666667$$

$\therefore$ Produces

$$\frac{25 \text{ mol}}{\text{L}} \Big| \, 0.6667 \, \Big| \, \frac{}{2}$$

$$= 8.333 \text{ mol/min } C$$

Sales $= (8.333)(40)$

$= \$333.33$

Exp $= \$125.00$

Profit ($/min) $208.33

Biomedical Modeling

Comparison of enzymatic protein digestion in stomach vs colon.

$V = 4.71\ L$

$v = 0.2\ L/hr$

$r = 1\ cm$

$L = 15\ m$

$$r = -\frac{V_m [P]}{K_m + [P]}$$

$V_m = 0.1\ \frac{gm}{L \cdot hr}$

$K_m = 0.5\ gm/L$

$[P_0] = 1\ gm/L$

Model stomach as MFR

colon as PFR

Calc. conversion

Stomach

$$\tau = \frac{[P_0]-[P]}{\left(\frac{V_m[P]}{K_m+[P]}\right)}$$

$$= \frac{([P_0]-[P])(K_m+[P])}{V_m[P]}$$

$$\tau V_m[P] = -[P]^2 + ([P_0]-K_m)[P] + [P_0]K_m$$

$$[P]^2 + (K_m + V_m\tau - [P_0])[P] - [P_0]K_m = 0$$

$$[P] = \frac{-b+\sqrt{b^2-4ac}}{2a}$$

$a = 1$

$b = (K_m + V_m\tau - [P_0])$

$c = -K_m[P_0]$

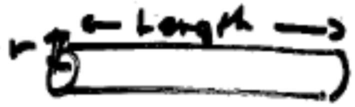
$\tau = \frac{4.71\ L}{0.2\ L/hr} = 23.5\ hr$

$$= 0.2388\ \frac{g}{L}$$

$$X = 1 - \frac{[P]}{[P_0]} = 0.7612$$

$$= 76.12\%$$

Colon



$$V = \pi r^2 (\text{Length})$$

$r = 1\,cm$ $\quad$ $\text{length} = 15\,m$

$$V = \frac{\pi\, 1^2\, \cancel{cm^2}}{} \Big| \frac{15\,\cancel{m}}{} \Big| \frac{\cancel{m^2}}{100^2\,\cancel{cm^2}} \Big| \frac{1000\,L}{\cancel{m^3}}$$

$$= 4.71\,L$$

$$\tau = \frac{V}{v} = 23.55\,hr$$

$$\frac{d[P]}{dt} = \frac{V_m [P]}{K_m + [P]} \Rightarrow \tau = \frac{K_m}{V_m} \ln \frac{[P_0]}{[P]} + \frac{1}{V_m}([P_0] - [P])$$

Iterative soln (Guess [P], calc τ, compare)

$[P_0] = 0.2388\ g/L$

P	τ_{calc}
0.2	1.27
0.1	5.74
0.01	18.15
0.005	21.67
0.003	24.24
0.0034	23.61
0.00393	23.56 ✓

$$\underline{\underline{X = .99657}}$$