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[illegible] (31/10/12)

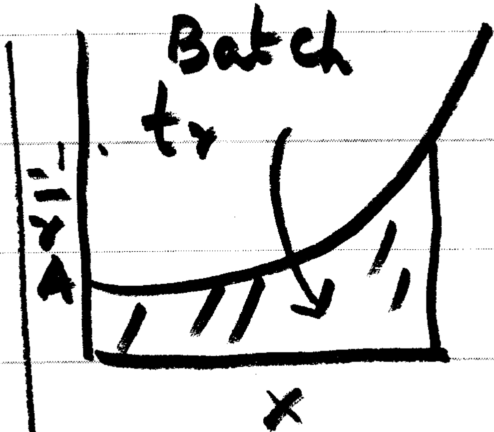
Advanced Reaction Engineering.

Design Equations

31 Oct 2012
1030-1130.

Design Equations

Batch: $t_r = N_{A0} \int_0^x \frac{dx}{-r_A \cdot V}$

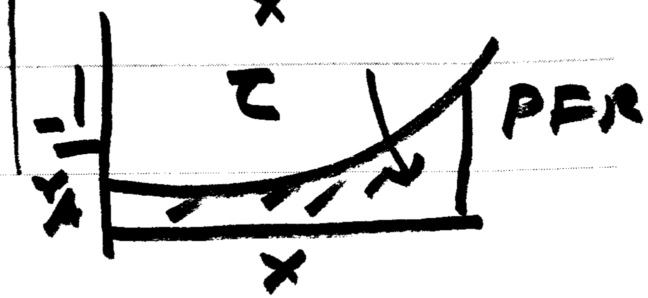


For constant volume batch

$$t_r = C_{A0} \int \frac{dx}{-r_A}$$

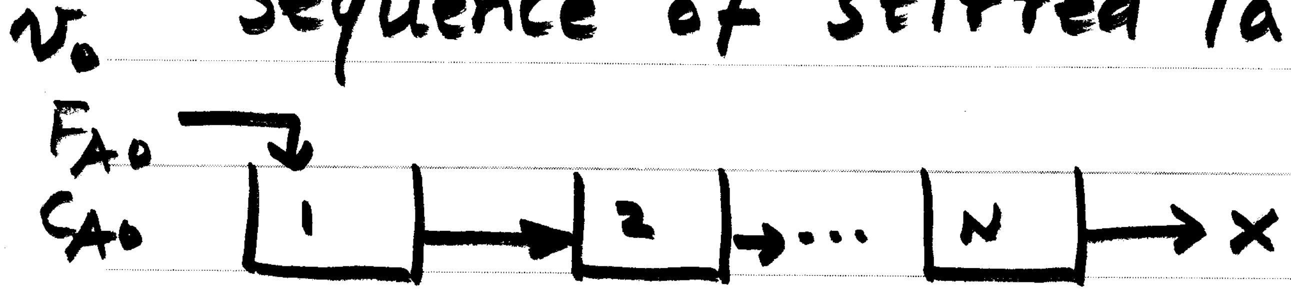
CSTR $\tau = \frac{C_{A0}\, x}{-r_A}$

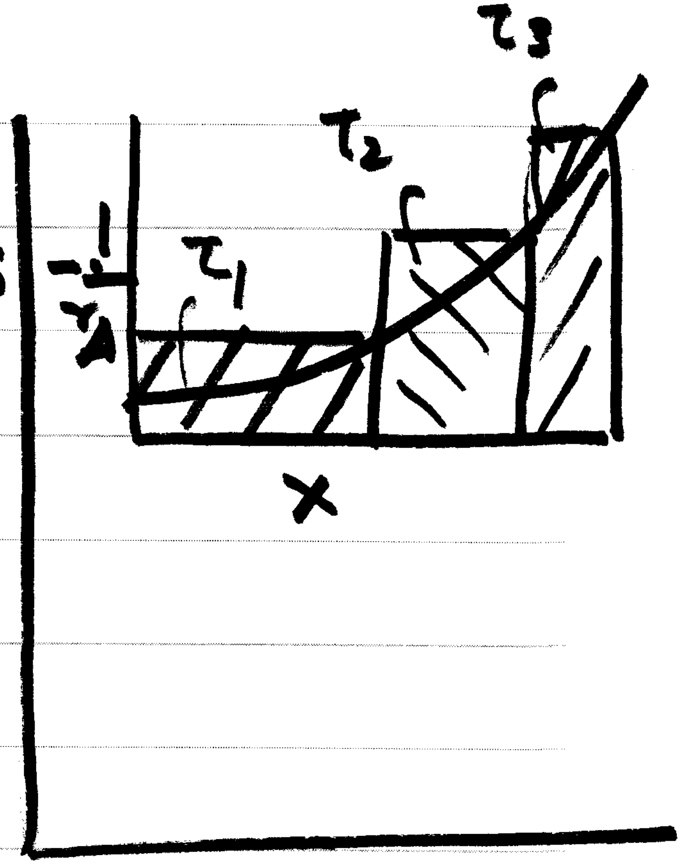
Plug flow: $\tau = C_{A0} \int \frac{dx_A}{-r_A}$



DESIGN EQUATIONS

Sequence of Stirred Tanks





$$V_1 = \frac{F_{A0} X_1}{-r_{A1}} \; ; \quad \tau_1 = \frac{C_{A0} X_1}{-r_{A1}}$$

$$V_2 = \frac{F_{A0}(X_2 - X_1)}{-r_{A2}} \; ; \quad \tau_2 = \frac{C_{A0}(X_2 - X_1)}{-r_{A2}}$$

$$V_N = \frac{F_{A0}(X_N - X_{N-1})}{-r_{AN}} \; ; \quad \tau_N = \frac{C_{A0}(X_N - X_{N-1})}{-r_{AN}}$$

$$aA + bB = cC + dD$$

Expressing C_A as function of X_A

Gas phase reactions. Batch Systems

$$pV = Z N_t R T$$

$$p_0 V_0 = Z_0 N_{t_0} R T_0.$$

$$\frac{V}{V_0} = \frac{Z}{Z_0} \frac{N_t}{N_{t_0}} \frac{\cancel{R}}{\cancel{R}} \frac{T}{T_0}$$

$$\frac{V}{V_0} = \left(1 + y_{A0} X_A \delta_A\right) \frac{T}{T_0} \frac{P_0}{P} \frac{Z}{Z_0}$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1 - X_A)}{V_0 (1 + y_{A0} X_A \delta_A) \frac{T}{T_0} \frac{Z}{Z_0} \frac{P_0}{P}}$$

$$C_A = \frac{C_{A0}(1 - X_A)}{(1 + y_{A0} X_A \delta_A)} \frac{T_0}{T} \frac{P}{P_0} \frac{Z_0}{Z}$$

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - N_{A0} X_A \, b/a}{V}$$

$$= \frac{N_{B0} - N_{A0} X_A \, b/a}{V_0 \left(1 + y_{A0} X_A \delta_A\right) \frac{T}{T_0} \frac{Z}{Z_0} \frac{P_0}{P}}$$

$$= \left[\frac{C_{B0} - C_{A0} X_A \, b/a}{\left(1 + y_{A0} X_A \delta_A\right)} \right] \frac{T_0}{T} \frac{Z_0}{Z} \frac{P}{P_0}$$

Similarly C_C and C_D

FLOW SYSTEM

$$p v = Z F_t R T$$

$$p_0 v_0 = Z_0 F_{t0} R T$$

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}} \frac{p_0}{p} \frac{T}{T_0} \frac{Z}{Z_0}$$

$$C_A = \frac{F_A}{v} \qquad \frac{F_{A0}(1-X_A)}{v}$$

$$C_A = \frac{C_{A0}(1-X_A)T_0}{(1+y_{A0}X_A\delta_A)T} \frac{Z_0}{Z} \frac{P}{P_0}$$

similarly

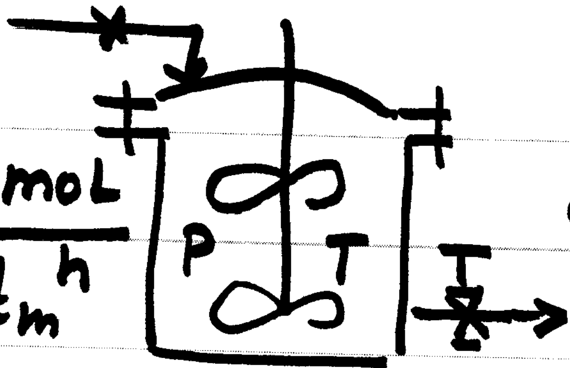
$$\left.\begin{matrix} C_B \\ C_C \\ C_D \\ C_I \end{matrix}\right\} \text{etc}$$

Q1

$F_{A0} = 1\ \frac{gmol}{h}$

$P = 1\ atm$

$T = 520C$



CSTR $\quad X_A = 0.5$

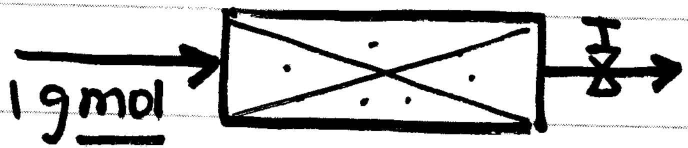
$$\underset{(A)}{\overset{(g)}{CH_3CHO}} = \underset{(B)}{\overset{(g)}{CH_4}} + \underset{(C)}{\overset{(g)}{CO}}$$

$$r_A = -k C_A^2$$

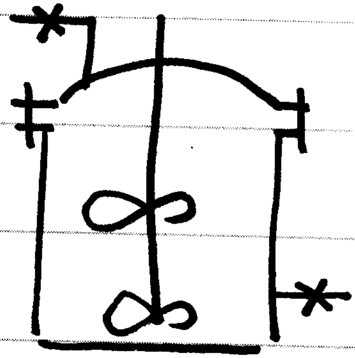
$F_{A0} = 1\ \frac{gmol}{L}$

$P = 1\ atm$

$T = 520C$



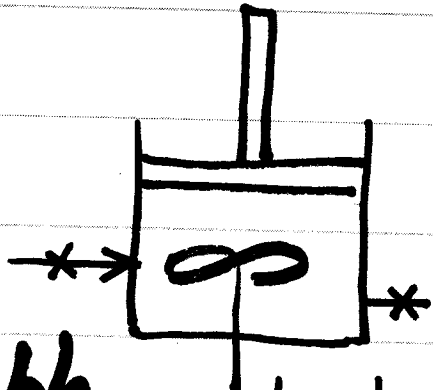
PFR



$P_0 = 1\ atm$

$T = 520$

CONSTAT VOLUNE BATCH



Variable Volume constant Pressure batch

CSTR.

$$\underset{A}{\overset{(g)}{CH_3CHO}} = \underset{B}{\overset{(g)}{CH_4}} + \underset{C}{\overset{(g)}{CO}}$$

stoichiometric Table

	IN	OUT
A	F_{A0}	$F_{A0}(1-x_A)$
B	$\cancel{F_{B0}}$	$F_{A0}\,x_A$
C	$\cancel{F_{C0}}$	$F_{A0}\,x_A$
	$F_{t0} = F_{A0}$	$F_t = F_{A0}(1+x_A)$

By gas Law

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}}\,\cancel{\frac{T}{T_0}}\,\cancel{\frac{Z}{Z_0}}\,\cancel{\frac{P_0}{P}} = \frac{\cancel{F_{A0}}(1+x_A)}{\cancel{F_{A0}}} = 1+x_A$$

$$\frac{v}{v_0} = 1 + X_A$$

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1 - X_A)}{v_0 (1+X_A)} = C_{A0} \frac{(1-X_A)}{(1+X_A)}$$

Design Eqn CSTR

$$V = \frac{F_{A0} X_A}{-r_A} \; * \; ;$$

$$= \frac{F_{A0} X_A (1+X_A)^2}{k C_{A0}^2 (1-X_A)^2} =$$

DATA

$P = 1\,atm$ $T = 520\,C$

$r_A = -k C_A^2$ (given)

$k = 0.33$ lit/gmol.s

$X_A = 0.5$ (given)

$$C_{A0} = P/RT = \frac{1.0\,atm}{(0.082\ lit.atm/gmol.K)\ 743} = 0.0154\ \frac{mol}{L}$$

$$V = \frac{F_{A0}\, x_A (1+x_A)^2}{k\, C_{A0}^2 (1-x_A)^2}$$

Putting numbers : $F_{A0} = 1$ mol/hr

$x_A = 0.5$

$C_{A0} = 0.0154$ mol/L

$$V = \frac{(1)(0.5)(1+0.5)^2}{(0.33)(3600)(1-0.5)^2} = 0.016\,M^3 = 16 \text{ LIT.}$$

$$\tau_{CSTR} = \frac{V}{v_0} = \frac{16}{(1.82)10^{-2}} = 878\,s$$

Integrating we get

$$V = \frac{F_{A0}}{k C_{A0}^2}\left[X_A + 4\ln(1-X_A) + \frac{4}{1-X_A} - 4\right]$$

Putting numbers

$F_{A0} = 1$ gmol/hr; $k = 0.33$ lit/gmol.s

$C_{A0} = 0.0154$ mol/L

$V = 6.3$ Lit; $\tau = \frac{V}{v_0} = \frac{6.3}{(1.82)10^{-2}} = 346$ s

Actual Residence Time PFR

$$\frac{dF_A}{dV} = r_A \quad ; \quad d\tau = \frac{dV}{v}$$

$$d\tau = \frac{dF_A}{v \cdot r_A} = -\left[\frac{F_{A0}}{v}\,\frac{dx}{r_A}\right] = \cancel{kC_{A0}}$$

$$r_A = -\frac{kC_{A0}^2 (1-x_A)^2}{(1+x_A)^2} \quad , \quad v = v_0 (1+x_A)$$

$$d\tau = \frac{F_{A0}}{v_0 (1+x_A)} \cdot \frac{(1+x_A)^2}{kC_{A0}^2 (1-x_A)^2}\, dx$$

$$d\tau = \frac{(1+x)}{k\,C_{A0}\,(1-x)^2}\,dx$$

$$\tau = \frac{1}{k\,C_{A0}}\left[\frac{2}{1-x} + \ln(1-x) - 2\right]$$

Putting numbers

$$\tau = \frac{1}{(0.33)(3600)(0.0154)}\left[\frac{2}{0.5} + \ln(0.5)\right]$$

τ = 261 seconds ACTUAL RESIDENCE TIME

PFR (CONSTANT PRESSURE)
ASSUMING NO PRESSURE DROP

Design Eqn

$$V = F_{A0} \int_0^{x_A} \frac{dx_A}{-r_A}$$

$$r_A = -k C_{A0}^2 \frac{(1-x_A)^2}{(1+x_A)^2}$$

$$V = F_{A0} \int_0^{x_A} \frac{(1+x_A)^2}{k C_{A0}(1-x_A)^2} \, dx_A \qquad x_A = 0.5.$$

CONSTANT VOLUME BATCH.

$\cancel{I/P} - \cancel{O/P} + \text{Gen} = \text{Acc.}$

$$\boxed{\frac{dN_A}{dt} = r_A V}$$

$$C_A = \frac{N_A}{V} = \frac{N_{A0}}{V_0}(1-x_A) = C_{A0}(1-x_A)$$

$$-N_{A0}\frac{dx_A}{dt} = -kC_A^2 V = -kC_{A0}^2(1-x_A)^2 V$$

$$N_{A0}\frac{dx_A}{dt} = kC_{A0}^2(1-x_A)^2 \cdot V$$

$$dt = \frac{N_{A0}}{V k C_{A0}^2 (1-x_A)^2} dx$$

$$dt = \frac{dx}{k C_{A0} (1-x)^2}$$

$$\boxed{t_r = \left(\frac{x_A}{1-x_A}\right) \frac{1}{k C_{A0}}}$$

$\therefore$

Putting numbers

$$t_r = \frac{0.5}{(0.33)(3600)(0.0154)(0.5)} = 0.0546 \text{ hrs}$$

$= 196$ Seconds

Pressure in Reactor Can be Calculated as

$$\frac{V}{V_0} = \frac{N_t}{N_{t_0}} \frac{T}{T_0} \frac{P_0}{P} \frac{Z}{Z_0}$$

$$\frac{P}{P_0} = \frac{N_t}{N_{t_0}} = 1+x$$

$$P = P_0(1+x) = P_0(1 \cdot 5)$$

constant Pressure Batch

$$\cancel{In} - \cancel{Out} + G = Acc$$

$$\frac{dN_A}{dt} = r_A V$$

$$\frac{V}{V_0} = \frac{N_t}{N_{t0}} \cancel{\frac{T}{T_0}} \cancel{\frac{z}{z_0}} \cancel{\frac{P_0}{P}}$$

$$\frac{V}{V_0} = (1 + X_A) \; ; \quad C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X_A)}{V_0(1+X_A)}$$

$$= C_{A0}(1-X_A)/(1+X_A)$$

$$-N_{A0}\frac{dx_A}{dt} = -kC_{A0}^2\,\frac{(1-x_A)^2}{(1+x_A)^2}\cdot V_0(1+x_A)$$

$$\boxed{\frac{dx_A}{dt} = kC_{A0}\,\frac{(1-x_A)^2}{(1+x_A)}}$$

Putting numbers

$t_r = 261\ s$

$$dt = \frac{(1+x_A)\,dx_A}{kC_{A0}(1-x_A)^2}$$

Same as PFR actual residence time

SOLN:

$$t_r = \frac{1}{kC_{A0}}\left[\frac{2}{1-x_A} + \ln(1-x_A)^{-2}\right]$$

COMPARISON OF EQUIPMENT.

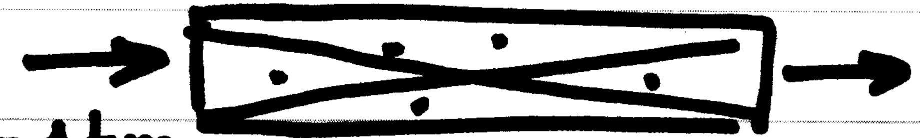
		(5) Time/Res
Constant vol. batch	$-kC_{A0}^{2}(1-X_A)^{2}$	200
Constant Presure batch	$-kC_{A0}^{2}(1-X_A)^{2}/(1+X_A)^{2}$	261
Constant Pressure PFR	$-kC_{A0}^{2}(1-X_A)^{2}/(1+X_A)^{2}$	261
Actual Residence time PFR		
Constant Pressure CSTR	$-\dfrac{kC_{A0}^{2}(1-X_A)^{2}}{(1+X_A)^{2}}$	878

Choosing equipment to give high rates gives low Res/time.

EFFECT OF PRESSURE DROP

$A \rightarrow B$

60 kg Catalyst



20 Atm $\qquad x_A = 0.865$

$$\frac{dP}{dW} = -0.2 \text{ atm/kg} \; ; \; r_A = -kC_A$$

1) What is x_A to be expected if PFR no pressure drop

2) If CSTR with no pressure drop

$$A \rightarrow B$$

$$\frac{dF_A}{dV} = r_A = -kC_A$$

$$\frac{v}{v_0} = \frac{F_t}{F_{t0}} \frac{T}{T_0} \left(\frac{P_0}{P}\right) \frac{Z}{Z_0} \quad \text{(gas Law)}$$

$$\frac{dP}{dW} = -0.2 \text{ atm/kg}$$

So that $P = P_0 - 0.2W$

$$\boxed{P/P_0 = 1 - 0.2W/P_0}$$

$$\frac{dx_A}{dW} = \alpha\left(1 - 0.2\frac{W}{P_0}\right)(1 - x_A)$$

$$\alpha = k / v_0 \rho \qquad \beta = \frac{0.2}{P_0}$$

$$\frac{dx_A}{1 - x_A} = \alpha\left(1 - 0.2\frac{W}{P_0}\right) dW$$

$$-\ln(1 - x_A) = \alpha\left(W - \beta W^2/2\right) + \text{Constant}$$

$x = 0 \quad W = 0$ so Constant $= 0$

$$\boxed{-\ln(1 - x_A) = \alpha\left(W - \beta W^2/2\right)}$$

From design Eqn

$$-\rho F_{A0} \frac{dx_A}{dW} = -k C_A \quad ; \quad \rho : \text{solid density}$$

$$C_A = F_A/v = \frac{F_{A0}(1-x_A)}{v_0 (P_0/P)}$$

$$C_A = C_{A0}(1-x_A)(1-0.2W/P_0)$$

$$\cancel{C_{A0}} \boxed{\frac{dx_A}{dW} = \frac{k \cancel{C_{A0}}}{v_0 \rho}(1-x_A)\left(1-0.2\frac{W}{P_0}\right)}$$

$$-\ln(1-X_A) = \alpha(W - \beta W^2/2)$$

Data: $X_A = 0.865$; $W = 60\text{kg}$,

$$\beta = 0.2/P_0 = 0.2/20 = 0.01$$

Putting numbers

$$-\ln(1-0.865) = \alpha\left[60 - 0.01\,\frac{3600}{2}\right]$$

$$\alpha = -\ln(0.135)/42 = 0.0476.$$

Plug Flow (No pressure drop)

$$-\ln(1-x_A) = \left(\frac{k}{v_0 \rho}\right) W$$

$\alpha =$

Note

$$\frac{dF_A}{dV} = r_A = -kC_A$$

$$-F_{A0}\frac{dx_A}{dV} = -kC_A$$

$$-F_{A0}\rho\frac{dx_A}{dW} = -kC_{A0}(1-x_A)$$

$$-\frac{dx_A}{\ } = -\frac{k}{v_0 \rho}(1-x_A)$$

$$\frac{dx_A}{dW} = \alpha(1-x_A)$$

$$\alpha = \frac{k}{v_0 \rho} = 0.0476$$

60 kg

Soln:

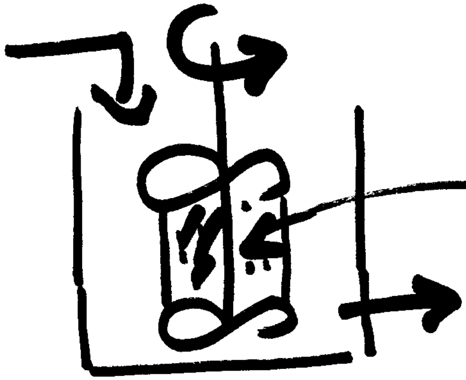
$$\boxed{-\ln(1-x_A) = \alpha W}$$

Putting numbers

$$-\ln(1-x_A) = (0.0476)\,60$$

$$\therefore x_A = 0.94$$

CSTR (NO PRESSURE DROP)



catalyst baskets

60 kg

$$r_A = -kC_A$$

$$V = \frac{F_{A0} X_A}{-r_A} = \frac{F_{A0} X_A}{k C_{A0} (1 - X_A)}$$

$$\left(\frac{W}{\rho}\right) = \frac{v_0 X_A}{k (1 - X_A)}$$

$$\frac{W k}{v_0 \rho} = \frac{X_A}{1 - X_A}$$

$W = 60$ kg

$\alpha = 0.0476$

$(\alpha = k / v_0 \rho)$

$$\frac{(60)}{0.0476} = \frac{X_A}{1 - X_A}$$

Pressure Drop in Process

$$SO_2 + \frac{1}{2} O_2 = SO_3$$

3000 ton/d SO_2 plant 4 stage

Short bed 0.25 M – 0.75 M, 70 TON

V_2O_5 catalyst, pressure drop 0.055 atm.

Power Consumption =

$$(0.055)\, 10^5 \frac{N}{M^2} \,(317\ m^3/s)\, / 0.7$$

Flow

blower efficiency

$$= \frac{1.75\ MW}{0.7} = 2.5\ MW$$

Pressure drop is a significant energy consumer