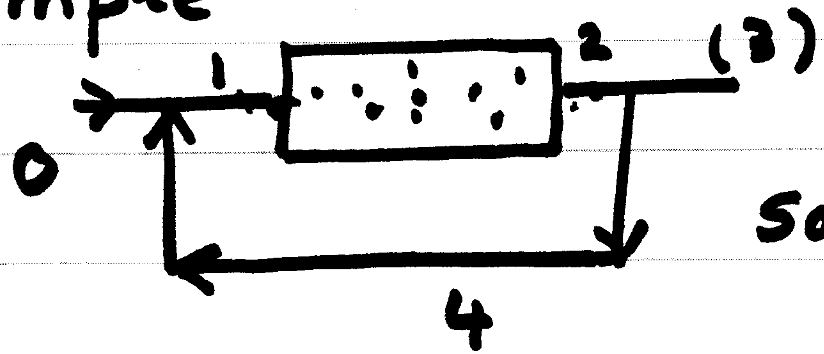
Advanced Reaction Engineering

Plug flow Recycle Reactors

Recycle Plug Flow Reactor

$aA + bB = cC + dD$

Example



Say $\underline{R} = 4 = \frac{F_{A4}}{F_{A3}}$

$x = 0.4$

	NO CATALYST	CATALYST	
F_{A0}	1	1.0	
F_{A1}	5.	3.4.	$\left(X_A = 1 - \frac{3.4}{5}\right) = 0.32$
F_{A2}	5	3.0.	$(X_A = 0.4)$
F_{A3}	1	0.6.	$(X_A = 0.4)$
F_{A4}	$R=0$ 4	2.4.	

(F_{A0}); $(R+1) F_{A0}$

1) We note that flow entering reactor in the absence of Reaction = $(R+1) F_{A0}$

2) So the basis of defining Conversion within recycle loop should $(R+1) F_{A0}$

3) Accordingly

$$X_1 = 1 - \frac{F_{A1}}{(R+1) F_{A0}} = 1 - \frac{3.4}{5} = 0.32$$

$$X_2 = 1 - \frac{F_{A2}}{(R+1) F_{A0}} = 1 - \frac{3}{5} = 0.4$$

We should expect that $X_2 = X_3$ since there is no Chemical Reaction between 2 and 3.

Using $(R+1) F_{A0}$ as basis makes it possible to retain the equality $X_2 = X_3$

$$\text{Per Pass Conversion} = \frac{F_{A1} - F_{A2}}{F_{A1}}$$

$$= (3.4 - 3.0)/3.4$$

$$= 0.117$$

Accordingly Recycle Reactors may give high overall conversion but per pass conversion can be kept quite low by suitable choices of process variables

In the absence of reaction

$$F_{A1} = (R+1)\, F_{A0}$$

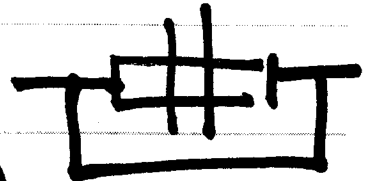
$$F_{A2} = (R+1)\, F_{A0}$$

$$F_{A3} = F_{A0}$$

$$F_{A4} = R\, F_{A3} = R\, F_{A0}.$$

Using flow through reactor in the absence of reaction as basis we can write the stoichiometric table

Stoichiometric Table Recycle PFR



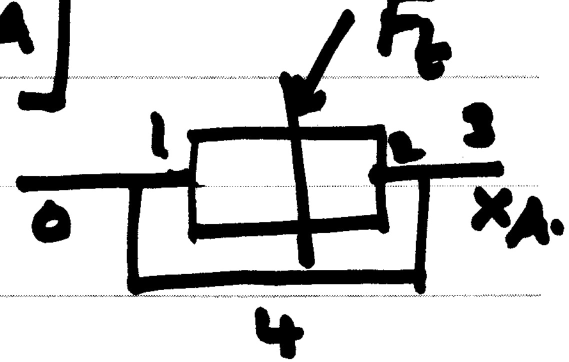
	IN	OUT
A	$(R+1)\,F_{A0}$	$(R+1)\,F_{A0}\,(1-X_A)$
B	$(R+1)\,F_{B0}$	$(R+1)\left[F_{B0}-\frac{b}{a}F_{A0}X_A\right]$
C	$(R+1)\,F_{C0}$	$(R+1)\left[F_{C0}+\frac{c}{a}F_{A0}X_A\right]$
D	$(R+1)\,F_{D0}$	$(R+1)\left[F_{D0}+\frac{d}{a}F_{A0}X_A\right]$
I	$(R+1)\,F_{I0}$	$(R+1)\,F_{I0}$

$$F'_{t0}=(R+1)\,F_{t0}$$

$$F_t=(R+1)\,F_{t0}+(R+1)\,F_{A0}\,\delta_A X_A$$

$$\frac{F_t}{F_{t0}}=(R+1)\left[\underbrace{1+y_{A0}X_A\delta_A}\right]$$

$$\frac{F_t}{F_{t0}} = (R+1)\left[1 + y_{A0}\,\delta_A\, x_A\right]$$



where $\delta_A = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$

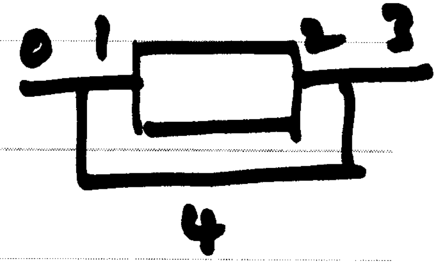
Taking material balance at '1'

$$F_{A0} + R\,\overbrace{F_{A0}(1 - X_3)}^{F_{A3}} = (R+1)\,F_{A0}\,(1 - X_1)$$

$$1 + R - R X_3 = R + 1 - (R+1) X_1$$

gives $\boxed{X_1 = \frac{R}{(R+1)} X_3}$

Per Pass Conversion



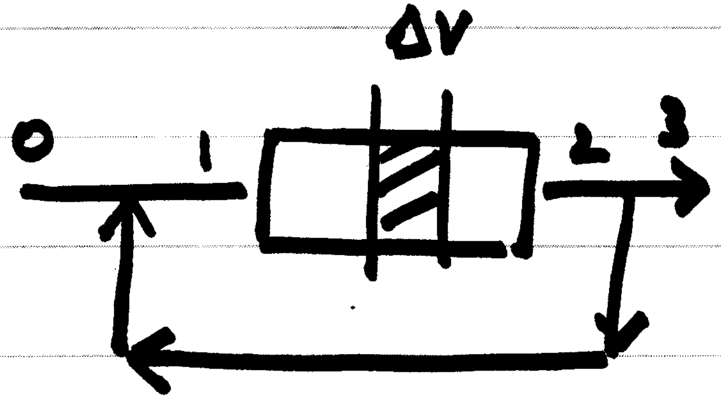
$$y_2 = \frac{F_{A1} - F_{A2}}{F_{A1}} = \frac{(R+1)\,F_{A0}\,(X_2 - X_1)}{(R+1)\,F_{A0}\,(1 - X_1)}$$

$$= \frac{X_2 - X_1}{1 - X_1} = \frac{X_2 - \frac{R}{R+1} X_2}{1 - \frac{R}{R+1} X_2}$$

$$y_2 = \frac{X_2\,(R+1)}{(R+1)(R+1-R\,X_2)} = \frac{X_2}{(R+1-R\,X_2)}$$

when R is large then y_2 is small

Design Equation for ~~Rey~~ Recycle PFR



$$\frac{dF_A}{dV} = r_A \checkmark \quad \text{PFR}$$

$$F_A = (R+1)\, F_{A0} (1 - X_A)$$

Substituting

$$-(R+1)\, F_{A0} \frac{dX_A}{dV} = r_A$$

$$V = (R+1)\, F_{A0} \int_{X_1}^{X_2} \frac{dX_A}{-r_A}$$

Design Equation

$$V = (R+1)\,F_{A0} \int_{X_1}^{X_2} \frac{dx_A}{-r_A}$$

where $X_1 = \frac{R}{(R+1)} X_2$ (Note $X_2 = X_3$)

Large R

$$\frac{V}{F_{A0}} = \lim_{R \to \infty} \frac{(R+1)\left\{ X_3 - \frac{R X_3}{R+1} \right\}}{(-r_A) \times \text{mean}\frac{(X_1 + X_2)}{2}}$$

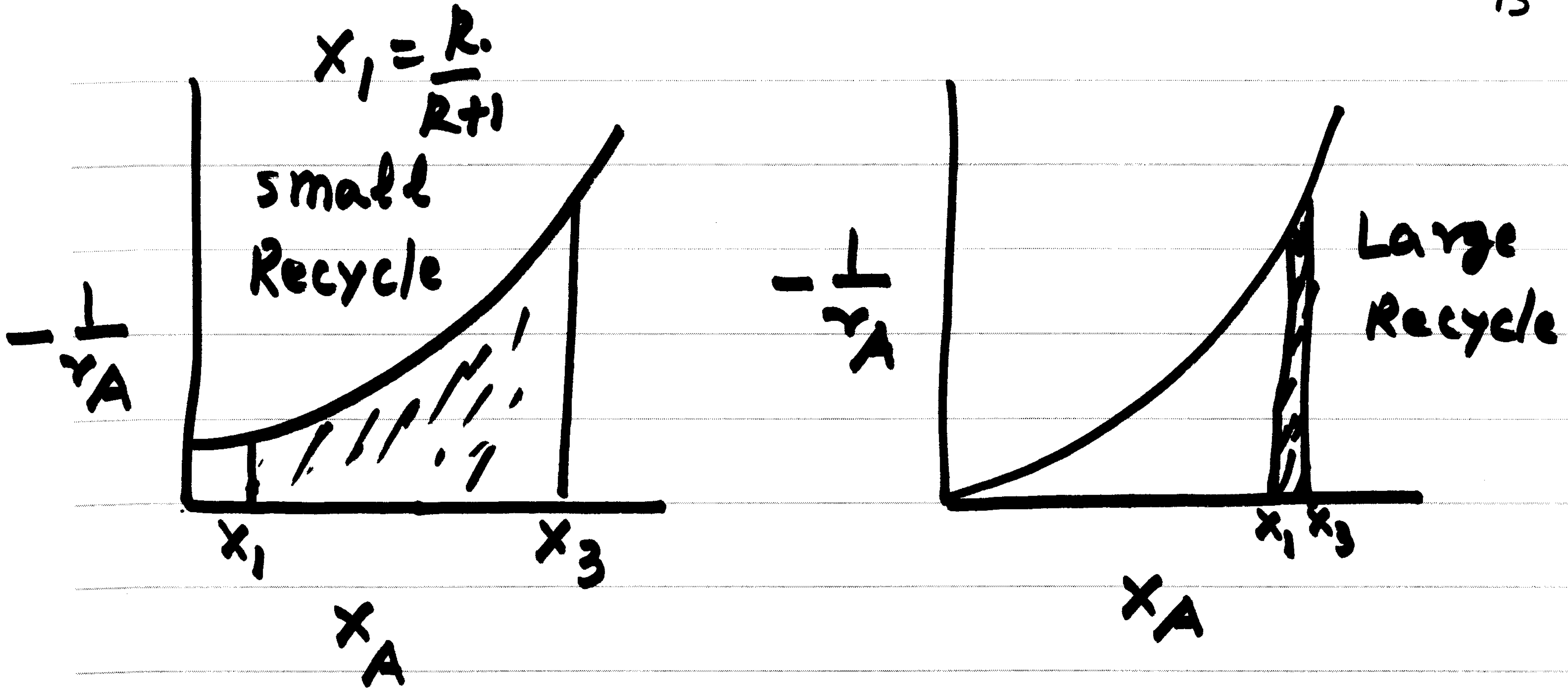
$$X_{mean} = \lim_{R \to \infty} \frac{\left[\frac{R X_3}{R+1} + X_3\right]}{2} = X_3$$

$$\frac{V}{F_{A0}} = \frac{X_3}{(-r_A)_{X_3}} \Rightarrow \text{same as CSTR}$$

So large recycle PFR behaves like CSTR

And when $R \to 0$ we get $\frac{V}{F_{A0}} = \int_0^X \frac{dx_A}{-r_A}$

which is PFR design Eqn.



It is clear from above figure that $R \rightarrow 0$ is PFR and $R \rightarrow$ infinity wehave CSTR

First order Reaction in R-PFR

$$\frac{V_R}{F_{A0}} = (R+1)\int_{X_1}^{X_3} \frac{dX_A}{-r_A} = (R+1)\int_{X_1}^{X_3} \frac{dX_A}{kC_{A0}(1-X_A)}$$

RXN: $A \rightarrow$ Products ; $r_A = -kC_A$

$$\frac{V_R}{F_{A0}} = \frac{(R+1)}{kC_{A0}} \Big[-\ln(1-X_A)\Big]_{\frac{R}{R+1}X_3}^{X_3}$$

$$k\tau_R = (R+1)\ln\left[\frac{1-\frac{R X_3}{R+1}}{1-X_3}\right]$$ where $\tau_R = V_R/v_0$

V_R – volume Recycle PFR

$$k\tau_p = -\ln(1-X_3)$$

NO MIXING PFR

$$k\tau_R = (R+1)\ln\left[\frac{1-\frac{R}{R+1}X_3}{1-X_3}\right]$$

R = 0 No Mixing PFR

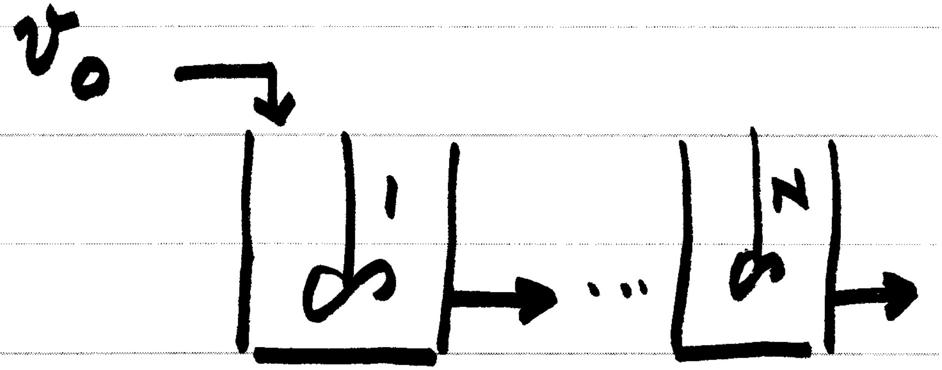
R infinity – CSTR

$$k\tau_N = N\left[\frac{1}{(1-X_N)^{1/N}}-1\right]$$

N = 1 ⇒ CSTR

N ⇒ Infinity PFR

N Tank Sequence



$$A \rightarrow B$$

$$F_{A0} - F_{A1} + r_{A1} V_1 = 0$$

$$c_{A0} - c_{A1} - k c_{A1} V_1 = 0.$$

$$\tau_1 = V_1 / v_0$$

$$c_{A1}(1 + k\tau_1) = c_{A0}$$

$$r_A = -k c_A$$

$$c_{A1} = c_{A0} / (1 + k\tau_1)$$

$$A \rightarrow B$$

similarly - $c_{A2} = \dfrac{c_{A1}}{(1 + k\tau_2)} = \dfrac{c_{A0}}{(1 + k\tau_1)(1 + k\tau_2)}$

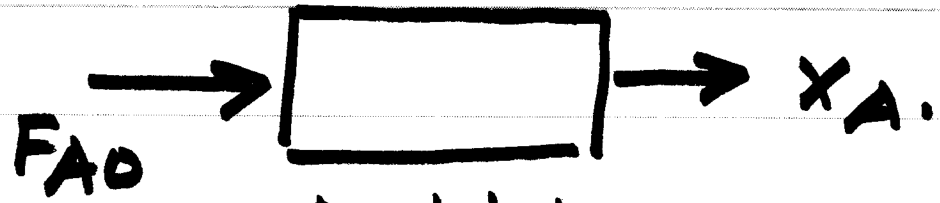
$$C_{AN} = \frac{C_{A0}}{\left(1 + k\frac{\tau}{N}\right)^N}$$

assuming $\tau_1 = \tau_2 \cdot = \tau_N = \tau/N$

$$\tau = \frac{N}{k}\left[\left(\frac{C_{A0}}{C_{AN}}\right)^{1/N} - 1\right]$$

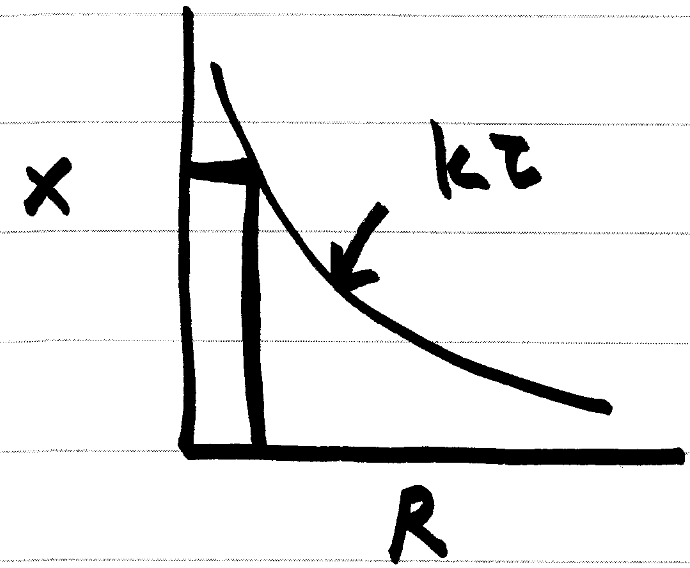
$$\tau = \frac{N}{k}\left[\frac{1}{(1-X_N)^{1/N}} - 1\right]$$

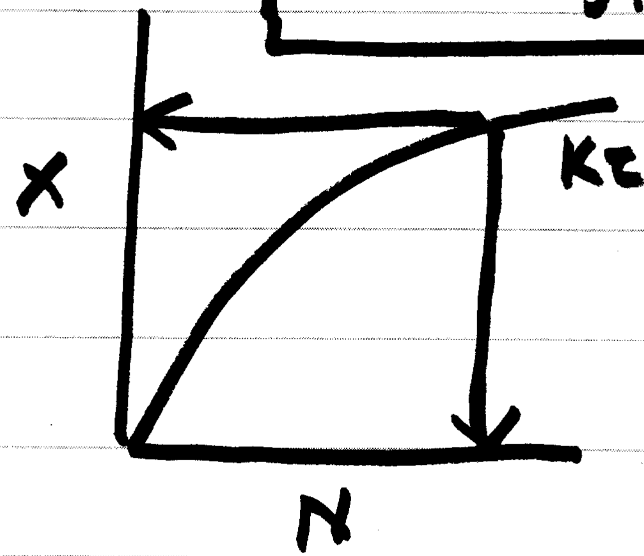
$$(k\tau_N) = N\left[\frac{1}{(1-X_N)^{1/N}} - 1\right]$$



Arbitary Vessel

> R + N are measures of Mixing.





x decreases
N → decreases
R → increases

From data for given Expt – x we can find R. Similarly N.

Uses of Recycle PFR

1) Recycle feeds into process products. So very useful in fermentations involving poly-culture

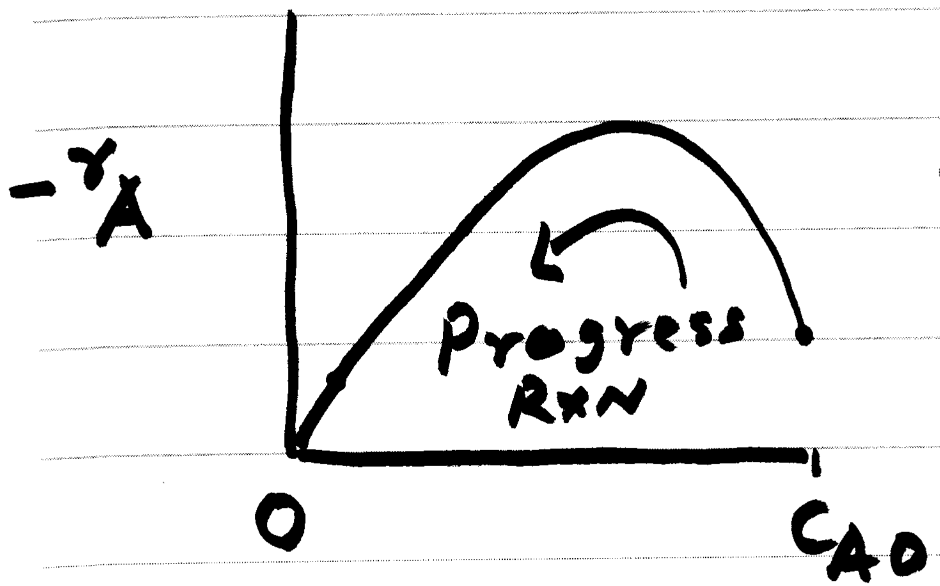
2) Recycle allows adjustment of velocities through reactor. So very valuble for Catalyst evaluation under varying Velocities

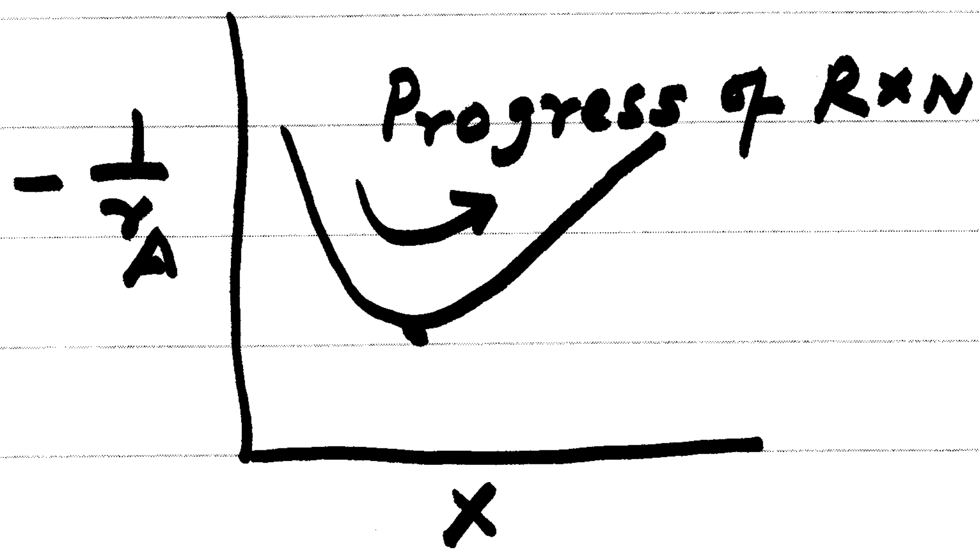
3) Recycle allows large velocities
so low per pass conversion
so essentially isothermal
operation possible even with
highly exothermic reactions
so can be used to get good
kinetic data

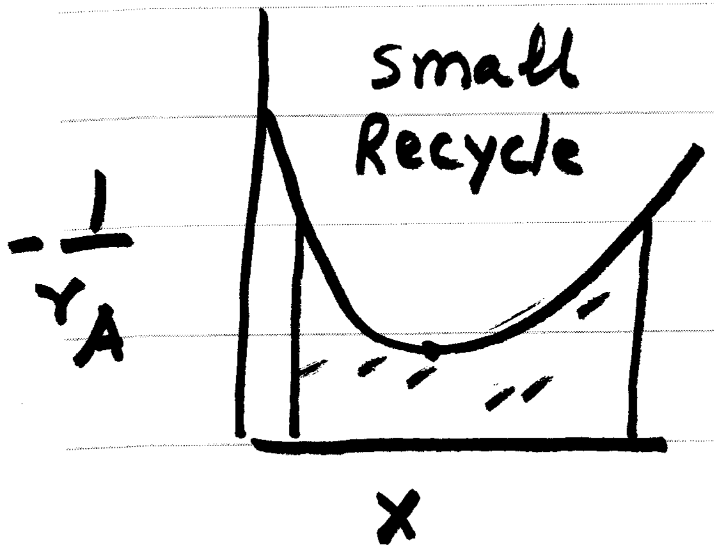
Auto Catalytic Reactions in Recycle PFR

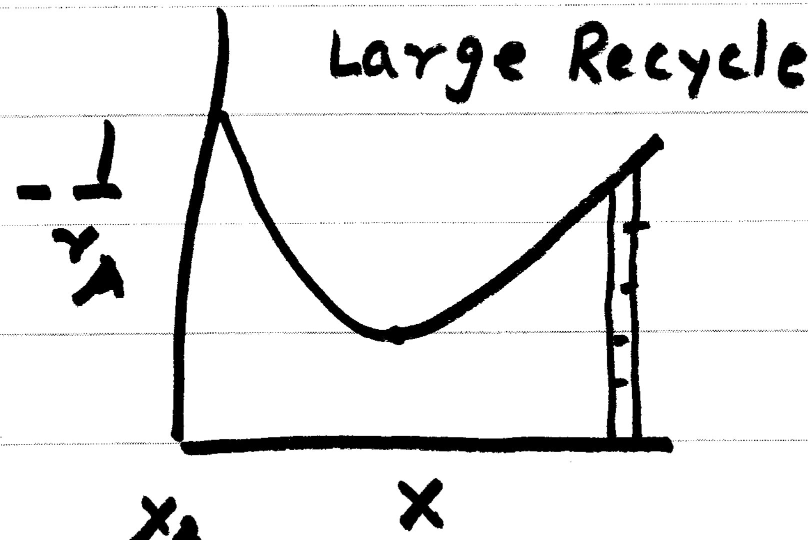
All Microbial Reactions/fermentation reactions are autocatalytic

$$A \rightarrow B \qquad r_B = k\, C_A\, C_B$$





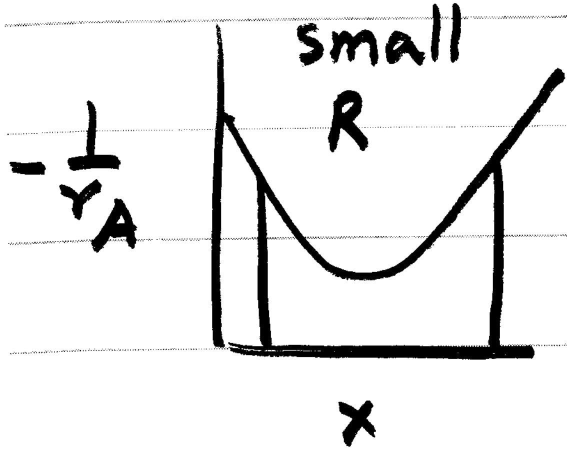


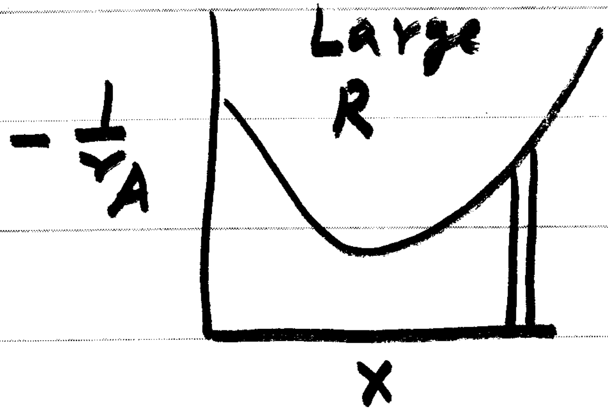


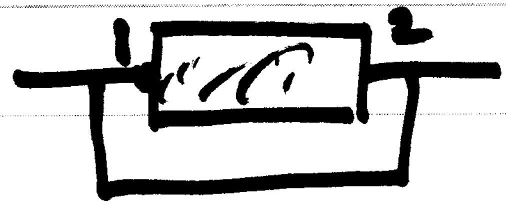
Design Eqn
$$\frac{V}{F_{A0}} = \underline{\underline{(R+1)}} \int_{X_1}^{X_2} \frac{dX}{-r_A}$$

It is clear from Eqn that as R increases (R+1) increases but as R increases area under curve decreases. For power law kinetics, autocat rxn an opt R exists.

optimum Recycle







We will show as a part of illustrative exercises that optimum Recycle R puts into reactor a feed whose $\left(-1/r_A\right)_{x1}$ is the average in the reactor

$$\left(-\frac{1}{r_A}\right)_{x1} = \frac{1}{(x_2 - x_1)} \int_{x_1}^{x_2} \frac{dx}{-r_A}$$

$$(C_A) = \frac{F_A}{v} = \frac{\cancel{(R+1)}\, F_{A0}\,(1-X_A)}{\cancel{(R+1)}\,(1+y_{A0}\, X_A\, \delta_A)\, v_0}$$

$$\frac{v}{v_0} = \frac{F_T}{F_{T0}}\, \cancel{\frac{T}{T_0}}\, \cancel{\frac{Z}{Z_0}}\, \cancel{\frac{P_0}{P}} = (R+1)\left[1+y_{A0}\, X_A\, \delta_A\right]$$

$$A \rightarrow B$$