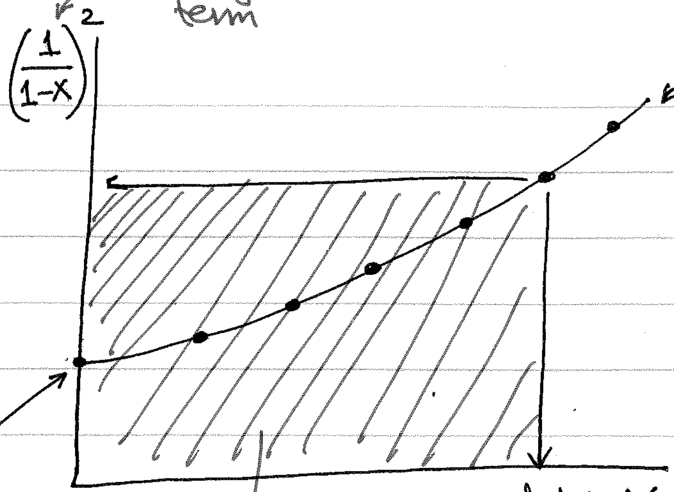
can be set

design term

$$\frac{v}{kC_{A0}}\left(\frac{1}{1-X}\right)^2$$

property of rxn. $\therefore$

can be set



curve is different from previous case

intercept $= \dfrac{v}{kC_{A0}}$

selected conversion X ← design term

Volume of reactor $= f(\text{cost})$

we assume that $\begin{Bmatrix}\text{volume} \\ \text{of reactor}\end{Bmatrix} \cong \begin{Bmatrix}\text{volume} \\ \text{of} \\ \text{rxn. mixture}\end{Bmatrix}$

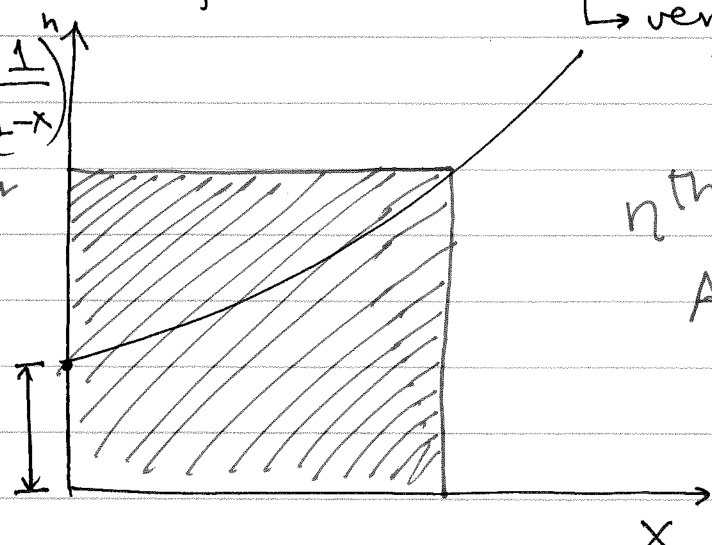
OR <u>we assume</u> $V_{reactor} = \text{scale-up } V_{rxn.}$

In general, for unimolecular rxns.

↳ very common in CSTRs

$$\frac{v}{kC_{A0}^{\,n-1}}\left(\frac{1}{1-X}\right)^n$$

$n \equiv$ order of rxn.



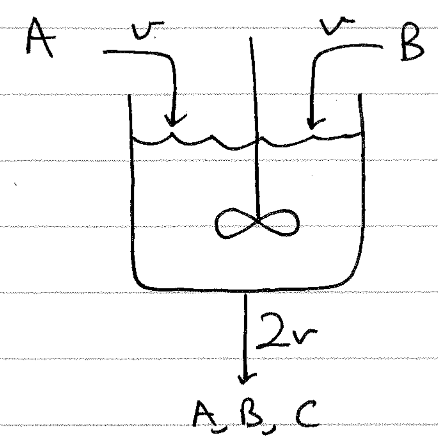
$\dfrac{v}{kC_{A0}^{\,n-1}}$

X

n^{th} order rxn

$A \longrightarrow B$

Consider 'multi' molecular systems:



* Why do A & B enter in separat[e] steams?
⇒ Think!

$$A + B \xrightarrow{k} C \qquad \& \quad -r_A = k C_A C_B$$

$$-r_A = -r_B = r_c \qquad \text{.... from stoichiometr[y]}$$

We assume volume change due to mixing is insignificant

General mole balance:

$$F_{io} - F_i = (-r_i) V \qquad \text{.... } i = A, B \text{ or } C \;\; (\text{for } C,\ r_c)$$

$$\therefore \quad F_{Ao} - F_A = (-r_A) V$$

$$F_{Bo} - F_B = (-r_B) V$$

$$-F_c = (+r_c) V$$

$$\therefore \quad F_c = r_c V \qquad \text{.... note the signs}$$

Algebraically, nothing changes.

$$\left.\begin{aligned} F_{A0} X_A &= (-r_A) V \\ F_{B0} X_B &= (-r_A) V \end{aligned}\right\} \text{given some variables, solve for others}$$

What about graphically?

$$V = \left(\frac{F_{A0}}{-r_A}\right) X_A$$

$$\therefore \quad V = \frac{C_{A0}\, v}{k C_A C_B} X_A$$

$$\therefore \quad V = \frac{v}{k}\left(\frac{C_{A0}}{C_A}\right)\left(\frac{1}{C_B}\right) X_A$$

$$X_A = \frac{v C_{A0} - 2 v C_A}{v C_{A0}} = \frac{C_{A0} - 2 C_A}{C_{A0}}$$

$$X_A = 1 - \frac{2 C_A}{C_{A0}}$$

$$\therefore \quad \frac{C_A}{C_{A0}} = \frac{1 - X_A}{2}$$

Similarly $\dfrac{C_B}{C_{B0}} = \dfrac{1 - X_B}{2}$

$$\therefore \quad V = \frac{\upsilon}{k}\left(\frac{2}{1-X_A}\right)\left(\frac{2}{1-X_B}\right)\left(C_{B0}^{-1}\right) X_A$$

$$\therefore \quad V = \frac{\upsilon}{k}\left[\frac{4}{(1-X_A)(1-X_B)}\right]\frac{1}{C_{B0}} X_A$$

$$\text{IIIly} \quad V = \frac{\upsilon}{k}\left[\frac{4}{(1-X_A)(1-X_B)}\right]\frac{1}{C_{A0}} X_B$$

$$\boxed{\therefore \quad V = \frac{\upsilon}{k\,C_{B0}}\left[\frac{4}{(1-X_A)(1-X_B)}\right]\cdot X_A}$$

Let us generalize this:

$$V = \frac{\upsilon}{\underbrace{k\,C_{B0}}_{\text{other reactants}}}\left[\frac{\overset{\text{fn. of split}}{4}}{\underbrace{(1-X_A)\,(1-X_B)}_{\text{no. of reactants}}}\right]\cdot X_A$$

For $\quad -r_A = k\,C_A\,C_B\,C_C$

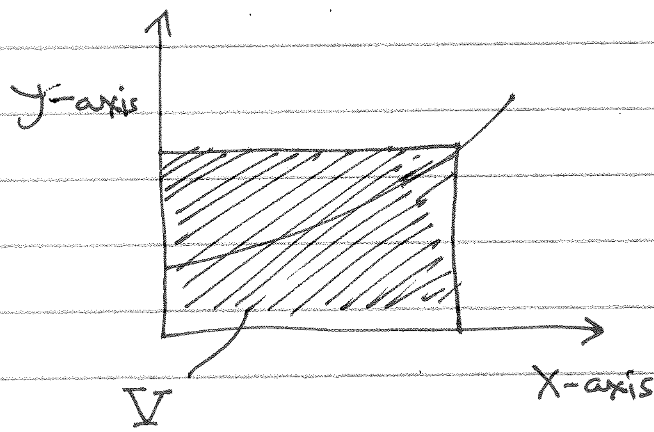
$$V = \frac{\upsilon}{k\,C_{C0}\,C_{B0}}\left[\frac{27}{(1-X_A)(1-X_B)(1-X_C)}\right]\cdot X_A$$

Generally,

$$\therefore \; V = \frac{v}{k \prod\limits_{i\neq j} C_{jo}} \left[\frac{n^n}{(1-X_A)\cdots(1-X_n)} \right] \cdot X_A$$

i.e.

$$\boxed{V = \underbrace{\frac{v}{k\prod\limits_{i\neq j}^{n} C_{jo}} \left[\frac{n^n}{\prod\limits_{i=A\ldots}^{n}(1-X_i)}\right]}_{\text{Y-axis}} \cdot \underbrace{X_A}_{\text{X-axis}}}$$



What about $-r_A = k\, C_A^a\, C_B^b \cdots C_p^p \cdots$

# of streams

$$V = \left(\frac{v}{k}\right)\left(\frac{1}{C_{Ao}^{a-1}}\right)\left(\frac{n}{1-X_A}\right)^a \times \left(\frac{1}{C_{Bo}}\right)^b \left(\frac{n}{1-X_B}\right)^b \cdots X_A$$

streams

$$\boxed{\therefore \; V = \frac{v}{k}\,\frac{1}{C_{Ao}^{a-1}} \prod_{j\neq i}^{n} \left(\frac{1}{C_{jo}}\right)^{\text{order}} \frac{n^{\sum \text{orders}}}{\prod\limits_{i=A\ldots}(1-X_i)^{\text{order}}} \cdot X_A}$$

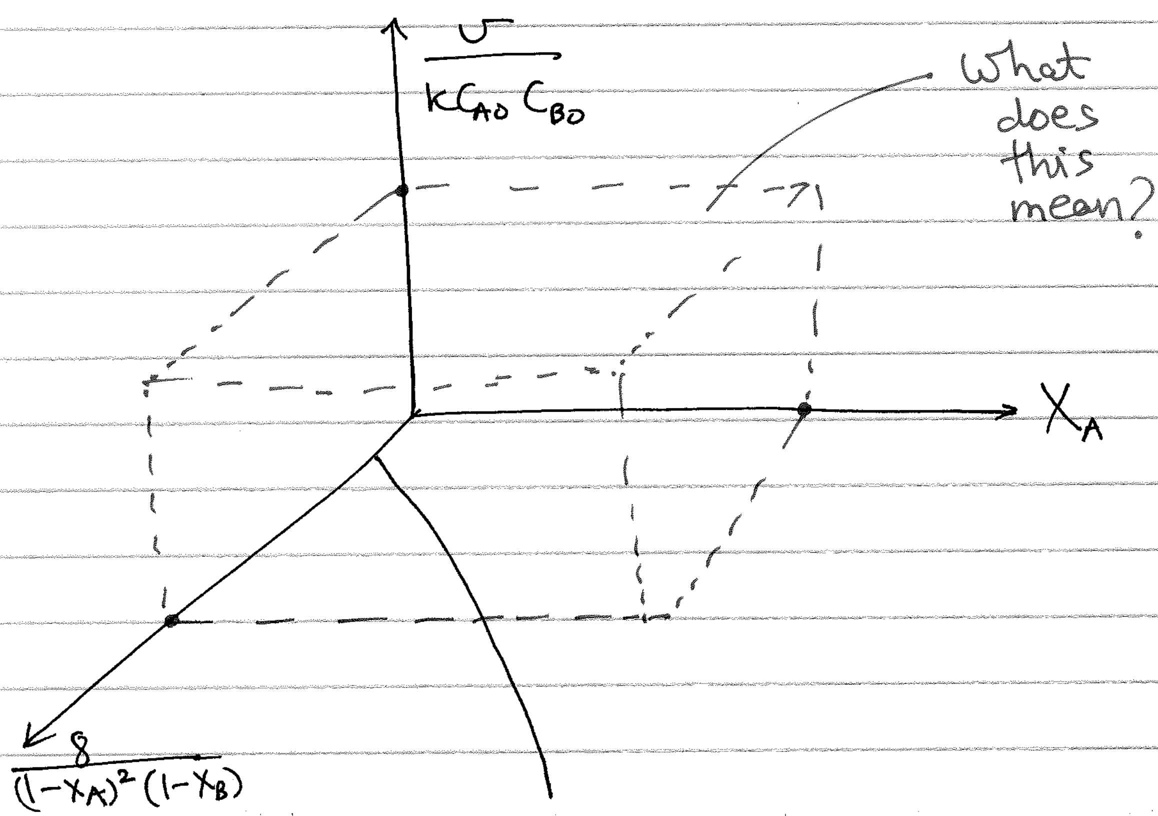
Consider $-r_A = k\,C_A^2\,C_B$ $(2A + B \rightarrow \text{products})$

$$\therefore\ V = \left(\frac{v}{k}\right)\left(\frac{1}{C_{A0}}\right)\left(\frac{1}{C_{B0}}\right)\frac{2^3}{(1-X_A)^2(1-X_B)}\ X_A$$

$$\therefore\ V = \underbrace{\left(\frac{v}{k\,C_{A0}\,C_{B0}}\right)}_{z\text{-axis}}\ \underbrace{\frac{8}{(1-X_A)^2(1-X_B)}}_{y\text{-axis}}\cdot \underbrace{X_A}_{x\text{-axis}}$$

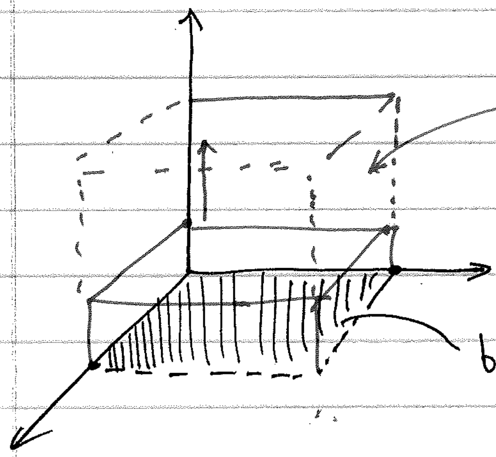
Also, from stoichiometry

$$X_B = \left(\frac{F_{A0}}{2F_{B0}}\right)X_A$$ .... we can calculate X_B easily



'Graphical tricks'

If you start @ high C_{A0}, C_{B0} but keep X_A & X_B at a fixed level



commensurate increase in volume

base unchanging since X_A & X_B fixed

Typical question: how high a C_{A0} & C_{B0} can I flow in until it becomes prohibitively expensive?

you could solve this in 2D as well but it isn't as easy to visualize

Design of PFRs

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

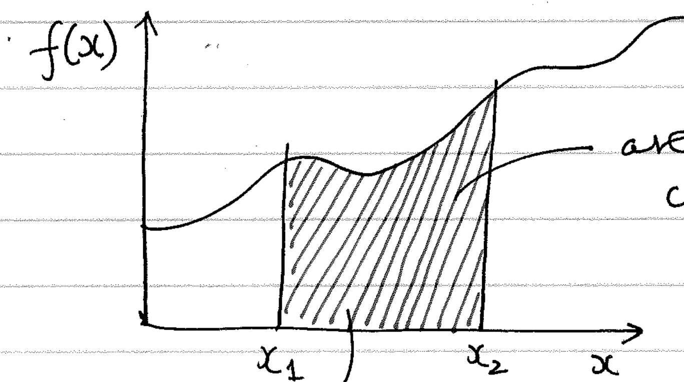
$$\therefore \quad dV = \frac{dF_A}{r_A}$$

$$\therefore \quad dV = -\frac{F_{A0}\, dX}{r_A}$$

$$\therefore \quad dV = \frac{F_{A0}\, dX}{(-r_A)}$$

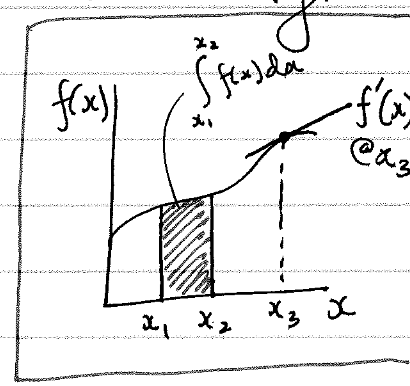
$$\boxed{\therefore \; V = \int \frac{F_{A0}}{(-r_A)} \cdot dX}$$

Let's look @ the definition of an integral

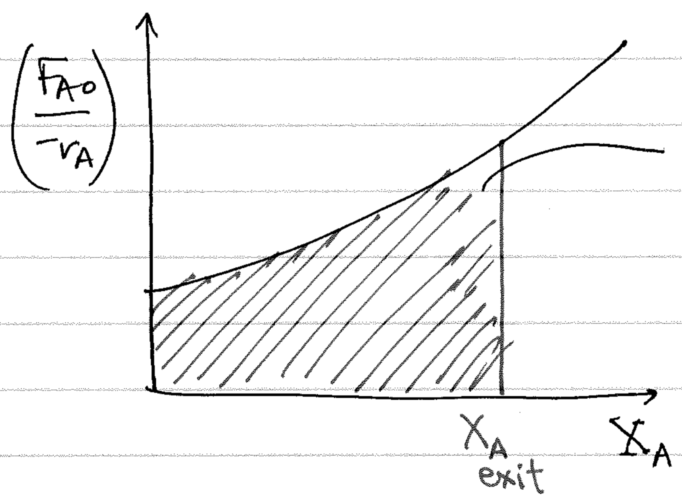


area under the curve ≡ integral

$$A = \int_{x_1}^{x_2} f(x)\, dx$$



$\therefore$



volume of a PFR

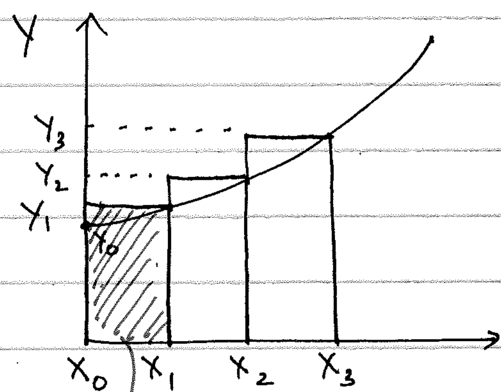
For PBR, it is $\left(\frac{F_{A0}}{-r_A'}\right)$ vs X_A

As always, $\frac{F_{A0}}{-r_A}$ can be rewritten in terms of X_A

→ you can plot the line by taking $X_A = 0, 0.1 \ldots$ & then calculating $\frac{F_{A0}}{-r_A}$

→ solve for area under the curve using **numerical methods**

Crude rectangles

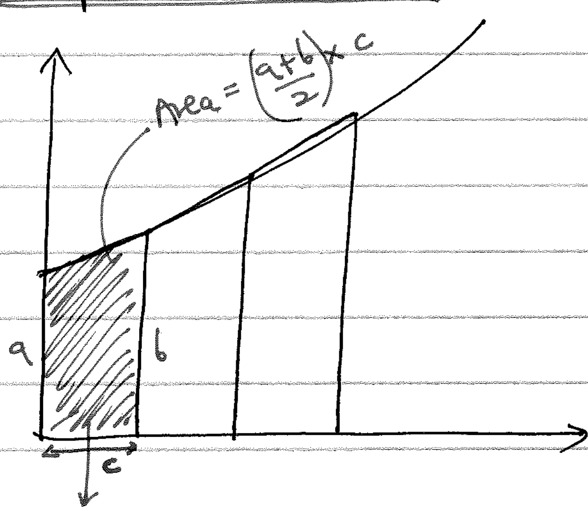


summation of areas of rectangles

X	Y (ht.)	ΔX (base)	areas
X_0	Y_0	—	—
X_1	Y_1	$X_1 - X_0$	$Y_1(X_1 - X_0)$
X_2	Y_2	$X_2 - X_1$	$Y_2(X_2 - X_1)$
X_3	Y_3	$X_3 - X_2$	$Y_3(X_3 - X_2)$
⋮	⋮	⋮	⋮

Total area = $\underbrace{\Sigma(\;)}$ ⇓ overestimate

Trapezoidal Rule



areas of trapezoids

X	Y	$\Delta X = c$	$\frac{a+b}{2}$	$\left(\frac{a+b}{2}\right)c$
X_0	Y_0	—	—	—
X_1	Y_1	$X_1 - X_0$	$\frac{Y_1+Y_0}{2}$	$(X_1 - X_0)\left(\frac{Y_0+Y_1}{2}\right)$
X_2	Y_2	$X_2 - X_1$	$\frac{Y_1+Y_2}{2}$	⋮
⋮	⋮	⋮	⋮	⋮

Area = Σ

more accurate than using rectangles

more accurate than trapezoidal rule

3 pt. wt.

Simpson's 1/3rd rule

X	Y	ΔX
X_0	Y_0	
X_1	Y_1	$\left(\frac{X_2 - X_0}{2}\right)\left(\frac{1}{3}\right)\left[Y_0 + 4Y_1 + 1 \cdot Y_2\right]$
X_2	Y_2	area of block
X_3	Y_3	
X_4	Y_4	$\left(\frac{X_5 - X_3}{2}\right)\left(\frac{1}{3}\right)\left[Y_5 + 4Y_4 + Y_3\right]$
$\vdots$	$\vdots$	

3 pts. @ a time

Total area $= \sum$

# of pts. should be a multiple of 3

↳ if not, perform Simpson's rule to maximum extent & then cap off with trapezoidal rule

same rule applies here

most accurate

4 pts. wt.

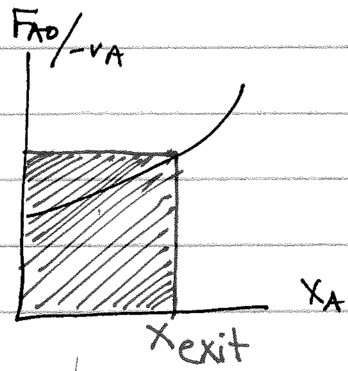
Simpson's 3/8th Rule

X	Y	ΔX
X_0	Y_0	
X_1	Y_1	$\left(\frac{X_3 - X_0}{3}\right)\left(\frac{3}{8}\right)\left[Y_0 + 3Y_1 + 3Y_2 + Y_3\right]$
X_2	Y_2	
X_3	Y_3	area of 1 block
X_4	Y_4	
$\vdots$	$\vdots$	

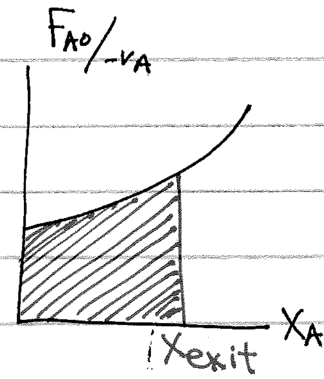
4 pts.

sum for total area

CSTR



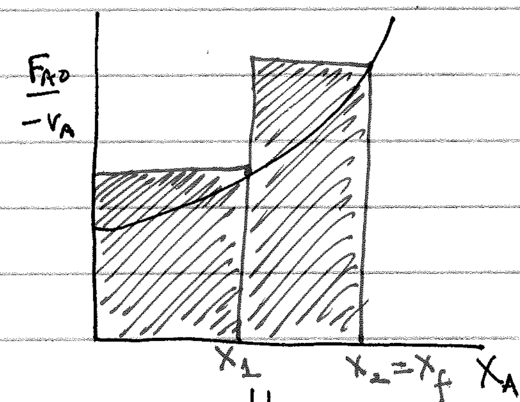
PFR



Which is more efficient? **PFR!**

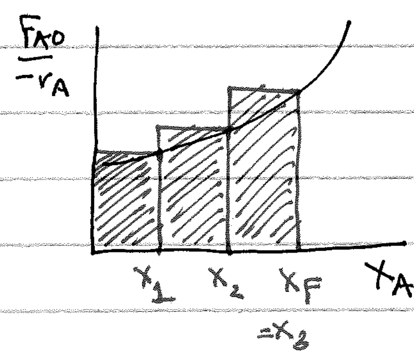
→ For the same volumes, PFRs achieve higher conversion.

In fact:

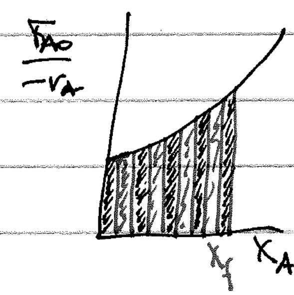


2 CSTRs in series

⇓



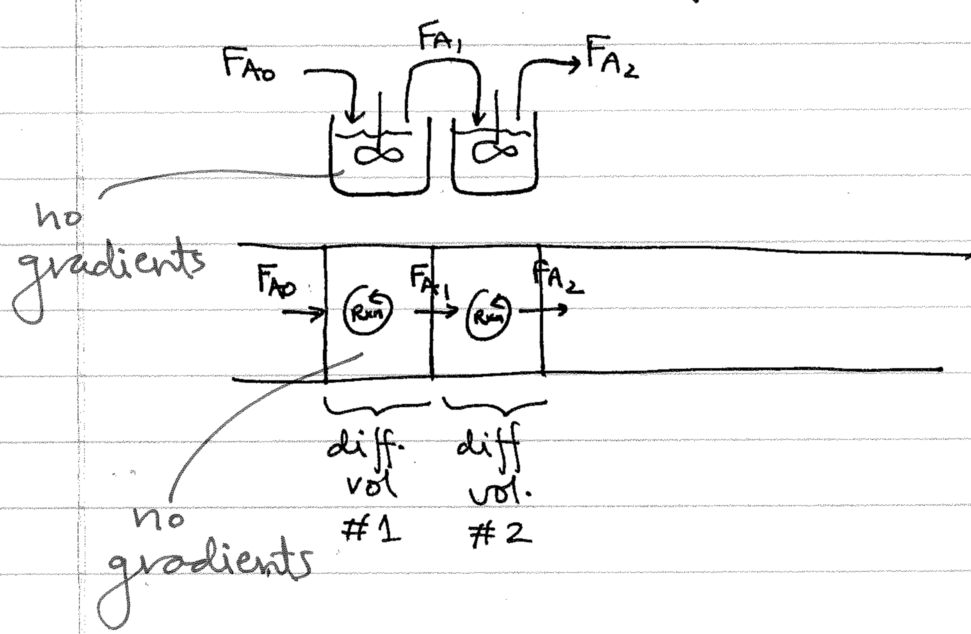
$\xrightarrow{\text{ultimately}}$



1 PFR = several CSTRs in series

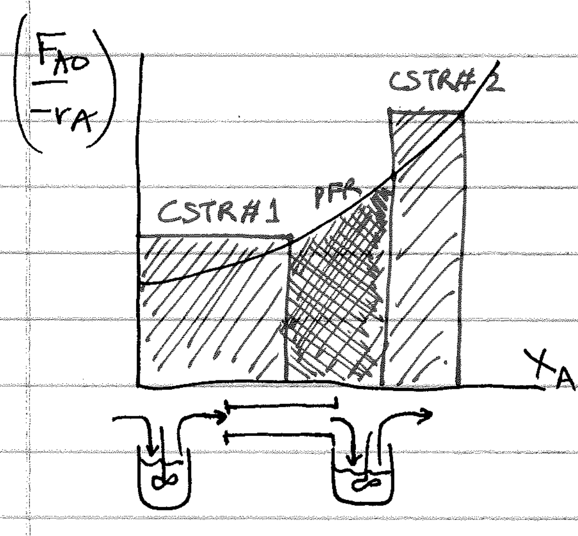
$\boxed{\text{As } n(\text{CSTR}) \to \infty \text{, the series approaches a true PFR}}$

<u>Remember how we defined a PFR:</u>

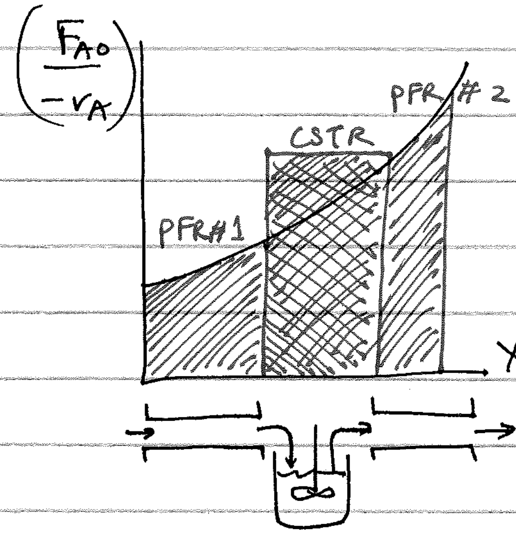


What about other combinations?

Straightforward!



CSTR – PFR – CSTR



PFR – CSTR – PFR

How to solve these problems?

→ What is the x-axis? $\underline{\underline{X_A}} \longrightarrow$ 1

→ What is the y-axis? $\frac{F_{A0}}{-r_A}$

$$\frac{F_{A0}}{-r_A} = \frac{C_{A0}\,v}{-r_A}$$ rate expression

Subst. X_A accordingly

If $-r_A = kC_A \Rightarrow \frac{F_{A0}}{-r_A} = \frac{v}{k}\left(\frac{C_{A0}}{C_A}\right) = \frac{v}{k}\left(\frac{1}{1-X_A}\right)$ ... if streams = 1 (in, out)

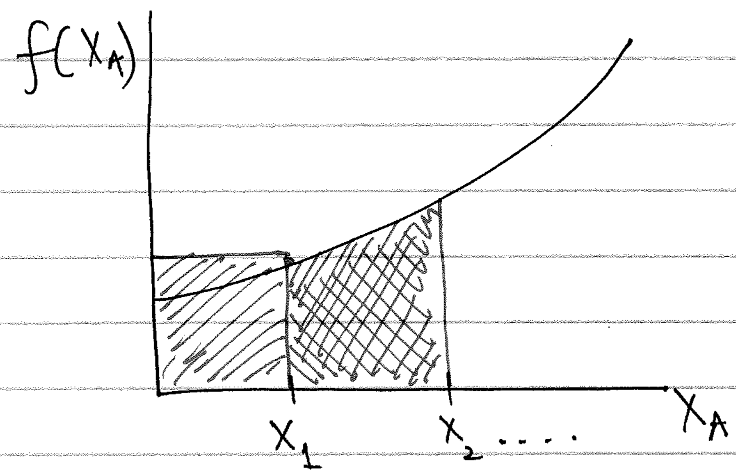
If $-r_A = kC_A^2 \Rightarrow +\frac{F_{A0}}{-r_A} = \frac{v}{k}\left(\frac{C_{A0}}{C_A}\right)^2 \frac{1}{C_{A0}} = \frac{v}{kC_{A0}}\left(\frac{1}{1-X_A}\right)^2$

If $-r_A = kC_AC_B \Rightarrow \frac{F_{A0}}{-r_A} = \frac{v}{kC_{B0}}\left(\frac{1}{1-X_A}\right)\left(\frac{1}{1-X_B}\right)$

Remember our formulas! PFRs have only 1 stream.

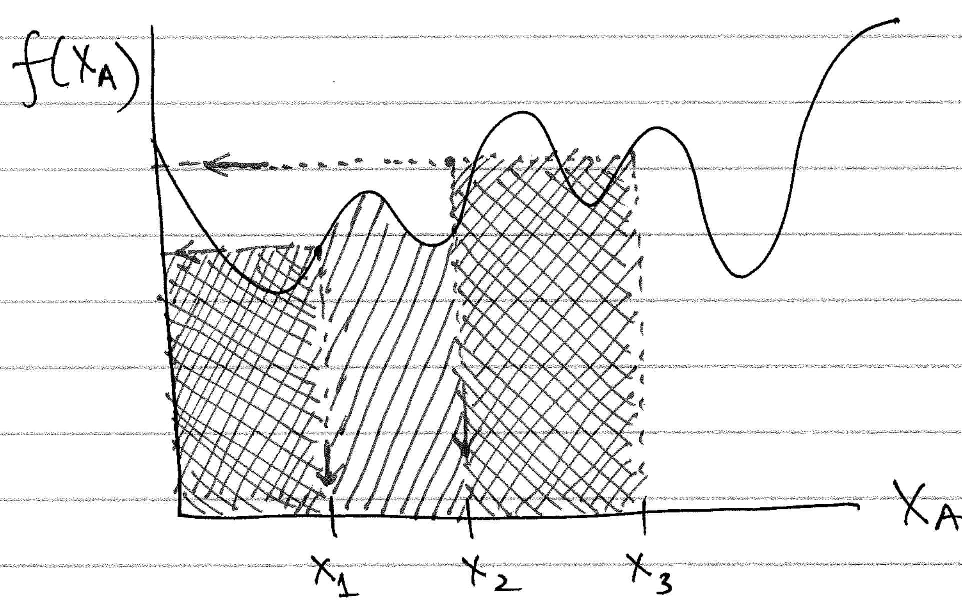
$\therefore$ → plot X_A

→ plot $\dfrac{v}{k\,C_{\text{initial of species}}} \times$ some fn. of X_A



Solve this graphically!

Even if $f(X_A)$ vs. X_A looks strange:



What setup (single or multiple reactors) is the best?