ChE 344
Reaction Engineering and Design

Lecture 2: Tues, Jan 11, 2022

Mole balance continued, Conversion, Levenspiel Plots, and Reactor Staging

Reading for today’s Lecture: Chapter 1, Chapter 2

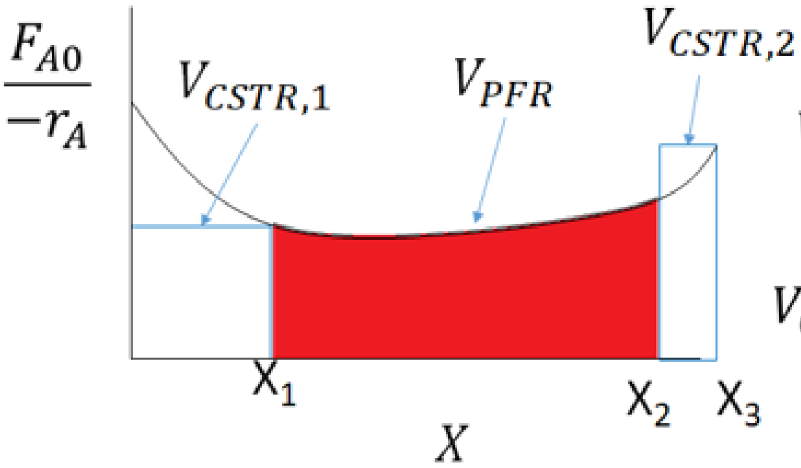
Reading for Lecture 3: Chapter 3

Lecture 2: Reactor Sizing Using Conversion
Related Text: Chapter 2

If there is only one significant reaction, and A is the limiting reactant we can use conversion.

Reactor	Conversion Definition	Mole balance	Mole Balance (aka Design Equation)
Batch	$X = \frac{N_{A0} - N_A}{N_{A0}}$	$N_A = N_{A0}(1 - X)$	$\frac{dX}{dt} = -\frac{r_A V}{N_{A0}}$
CSTR	$X = \frac{F_{A0} - F_A}{F_{A0}}$	$F_A = F_{A0}(1 - X)$	$V_{CSTR} = \frac{F_{A0}(X_{out} - X_{in})}{-r_A}$
PFR	$X = \frac{F_{A0} - F_A}{F_{A0}}$	$F_A = F_{A0}(1 - X)$	$V_{PFR} = \int_{X_{in}}^{X_{out}} \frac{-F_{A0}}{r_A} dX$
PBR	Same as PFR, plus uniform catalyst	$r_j' = \frac{dF_j}{dW}$	$W_{PBR} = \int_{X_{in}}^{X_{out}} \frac{-F_{A0}}{r_A'} dX$

Levenspiel Plots:



$$V_{PFR} = \int_{X_{in}}^{X_{out}} \frac{-F_{A0}}{r_A} dX$$

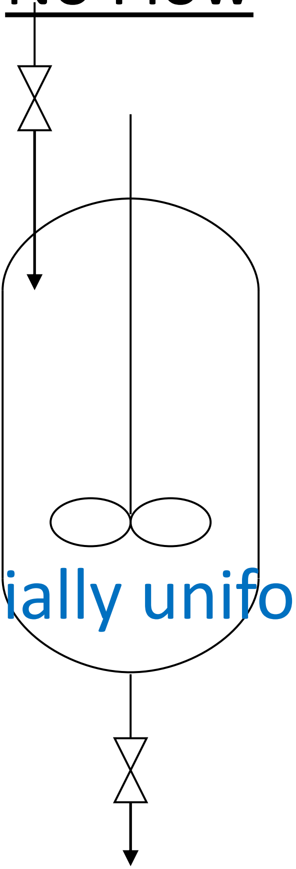
$$V_{CSTR} = \frac{F_{A0}(X_{out} - X_{in})}{-r_A}$$

Last time: The Generalized Mole Balance Equation

$$F_{j0} - F_j + \int_0^V r_j dV = \frac{dN_j}{dt}$$

Common types of reactors we introduced last time:

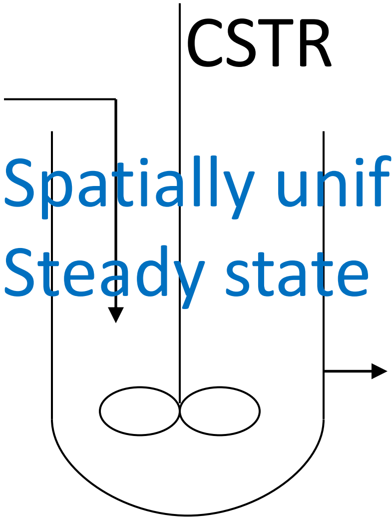
No Flow



Batch

Spatially uniform

Continuous Flow



CSTR

Spatially uniform,
Steady state

Plug flow

No radial variation,
steady state

Batch reactor design equation

- Not steady state
- Rate doesn't depend on position (makes these also sometimes called well-mixed reactors)
- No flows in or out

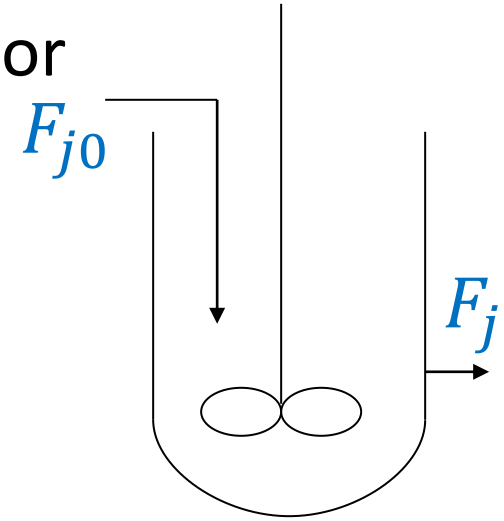
$$\cancelto{0}{F_{j0}} - \cancelto{0}{F_j} + \int_0^V r_j dV = \frac{dN_j}{dt}$$

$$\boxed{r_j V = \frac{dN_j}{dt}}$$

$$dt = \frac{dN_j}{r_j V} \qquad \int_0^{t_1} dt = \int_{N_{j0}}^{N_{j1}} \frac{1}{r_j V} dN_j$$

Constant/continuous stirred tank reactor (CSTR)

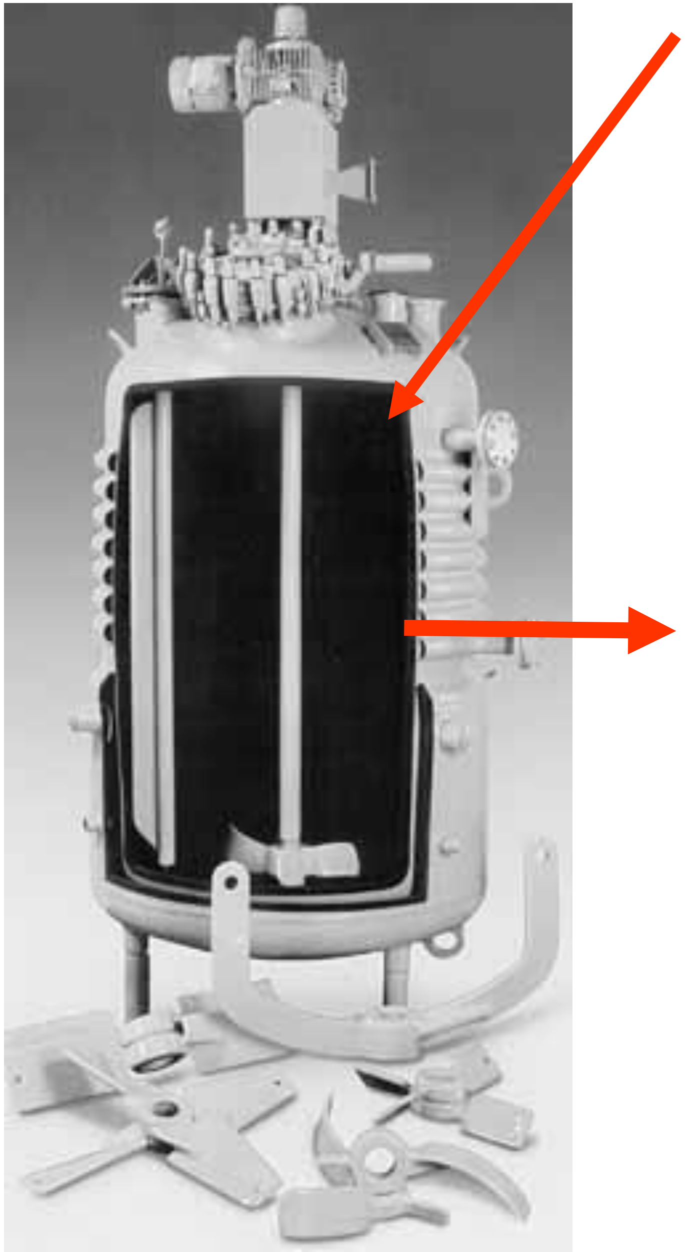
Inlet stream conc. are different than in reactor



All conc. at outlet and in reactor are the same

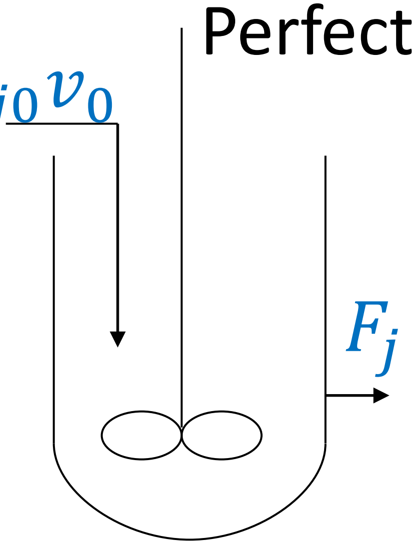
CSTR

Batch + Flow at Steady State = CSTR



Constant/continuous stirred tank reactor (CSTR)

Inlet stream conditions $F_{j0} = C_{j0} v_0$ are different than in reactor



All conditions at outlet and in reactor are the same

- Flow in and out (v is volumetric flow rate
- Well-mixed
- Steady state

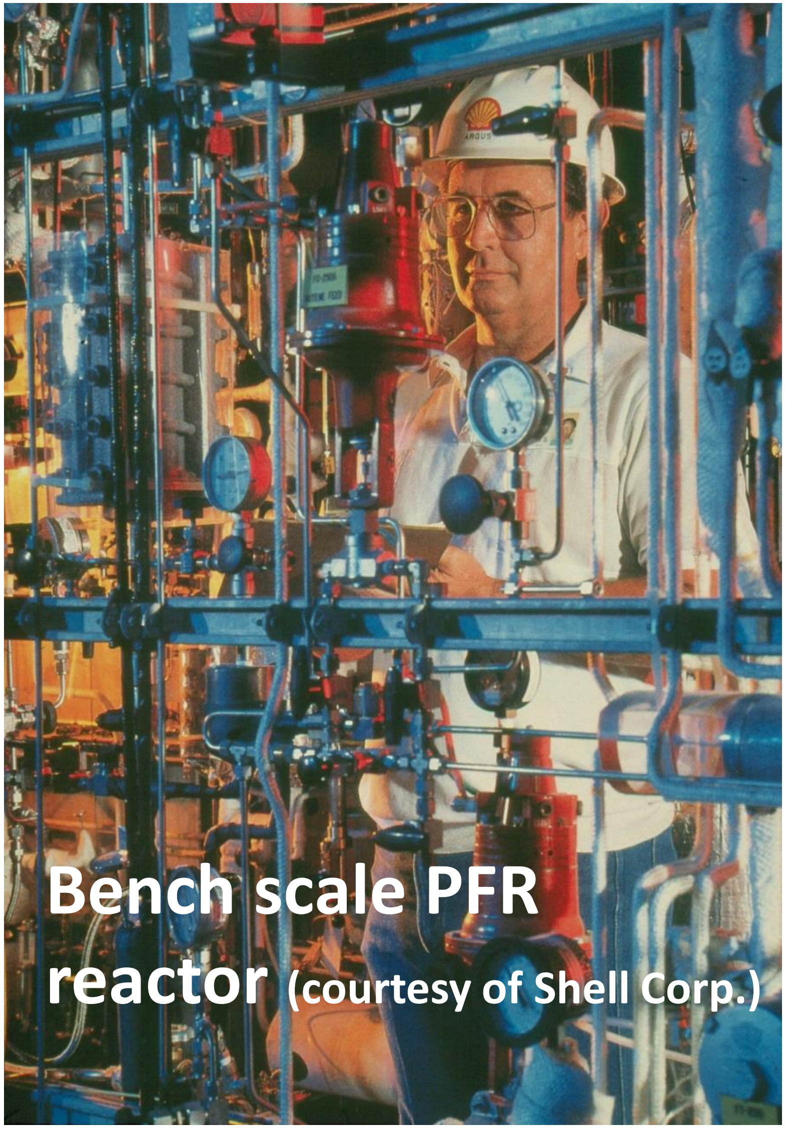
$$F_{j0} - F_j + \int_0^V r_j dV = \cancelto{0}{\frac{dN_j}{dt}}$$

$$F_{j0} - F_j + r_j V = 0$$

$$V_{CSTR} = \frac{F_{j0} - F_j}{-r_j}$$

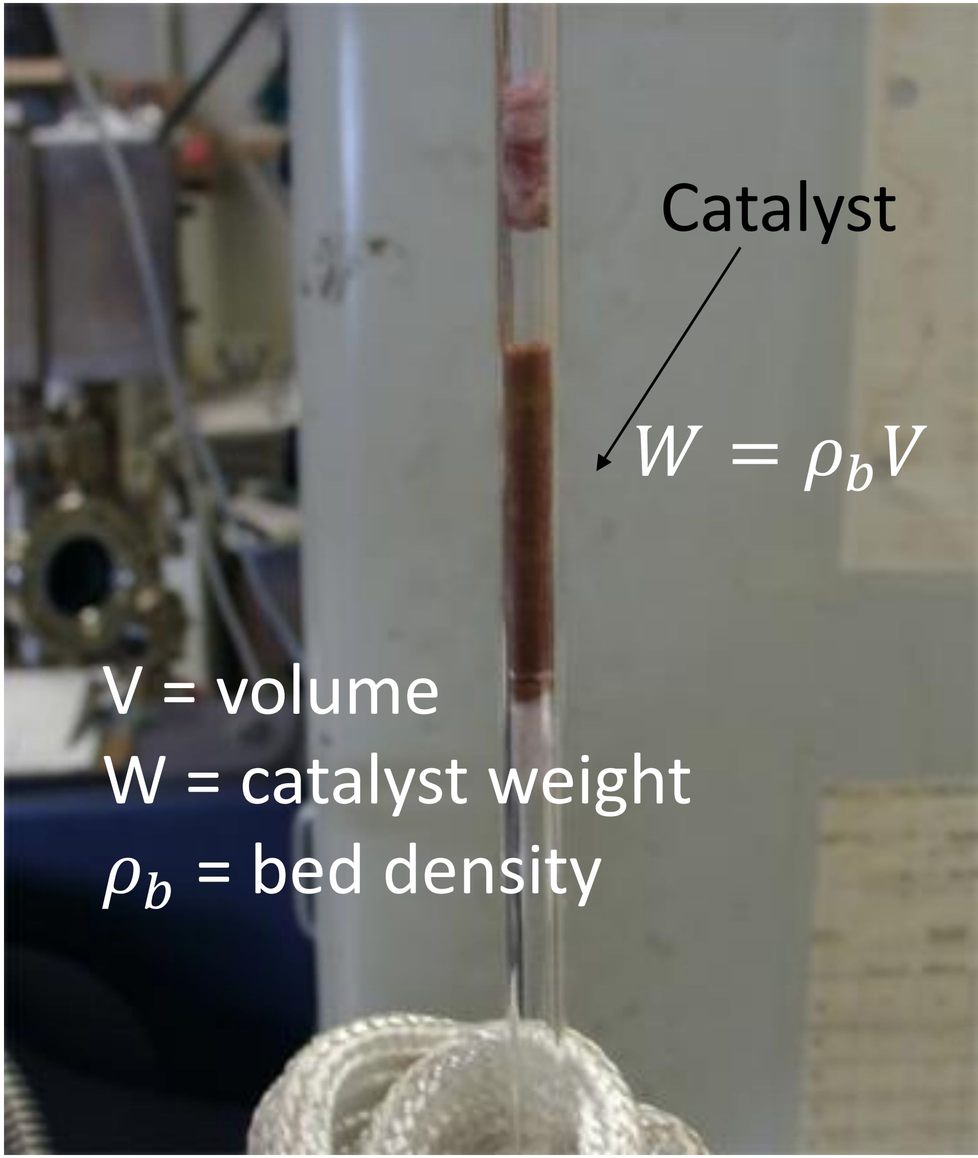
$$F_j = C_j v$$

Plug Flow Reactor (PFR)



Bench scale PFR reactor (courtesy of Shell Corp.)

Packed Bed Reactor (PBR)



Catalyst

$$W = \rho_b V$$

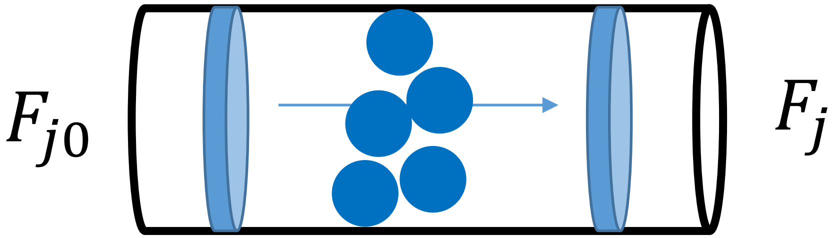
V = volume

W = catalyst weight

ρ_b = bed density

Plug flow reactor or packed bed reactor

- No radial variation
- No parabolic profile
- Each ΔV of fluid is treated as an ideal CSTR (steady state)

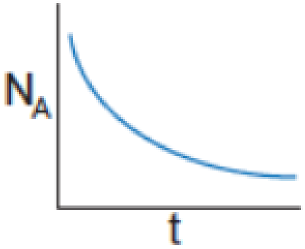
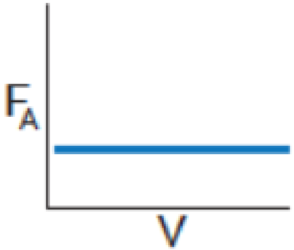
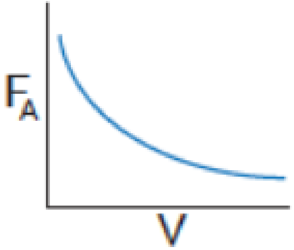


$$F_{j0} - F_j + \int_0^V r_j dV = \cancelto{0}{\frac{dN_j}{dt}}$$

$$F_{j,V} - F_{j,V+\Delta V} + r_j \Delta V = 0$$

$$r_j = \frac{dF_j}{dV}$$

Chapter 1 Summary: Reactor Mole Balances/Design Eqs

Reactor	Assumptions	Mole Balance	Reactant Profile
Batch	Spatially uniform, no inlet/outlet streams	$r_j V = \frac{dN_j}{dt}$	
CSTR	Spatially uniform, steady state	$V = \frac{F_j - F_{j0}}{r_j}$	
PFR	No radial variation, steady state	$r_j = \frac{dF_j}{dV}$	
PBR		$r_j' = \frac{dF_j}{dW}$	W is catalyst weight

Discuss with your neighbors or consider on your own:

If we think of a hippo’s stomach as a reactor, which would be the most appropriate reactor to use as a model?

A) CSTR

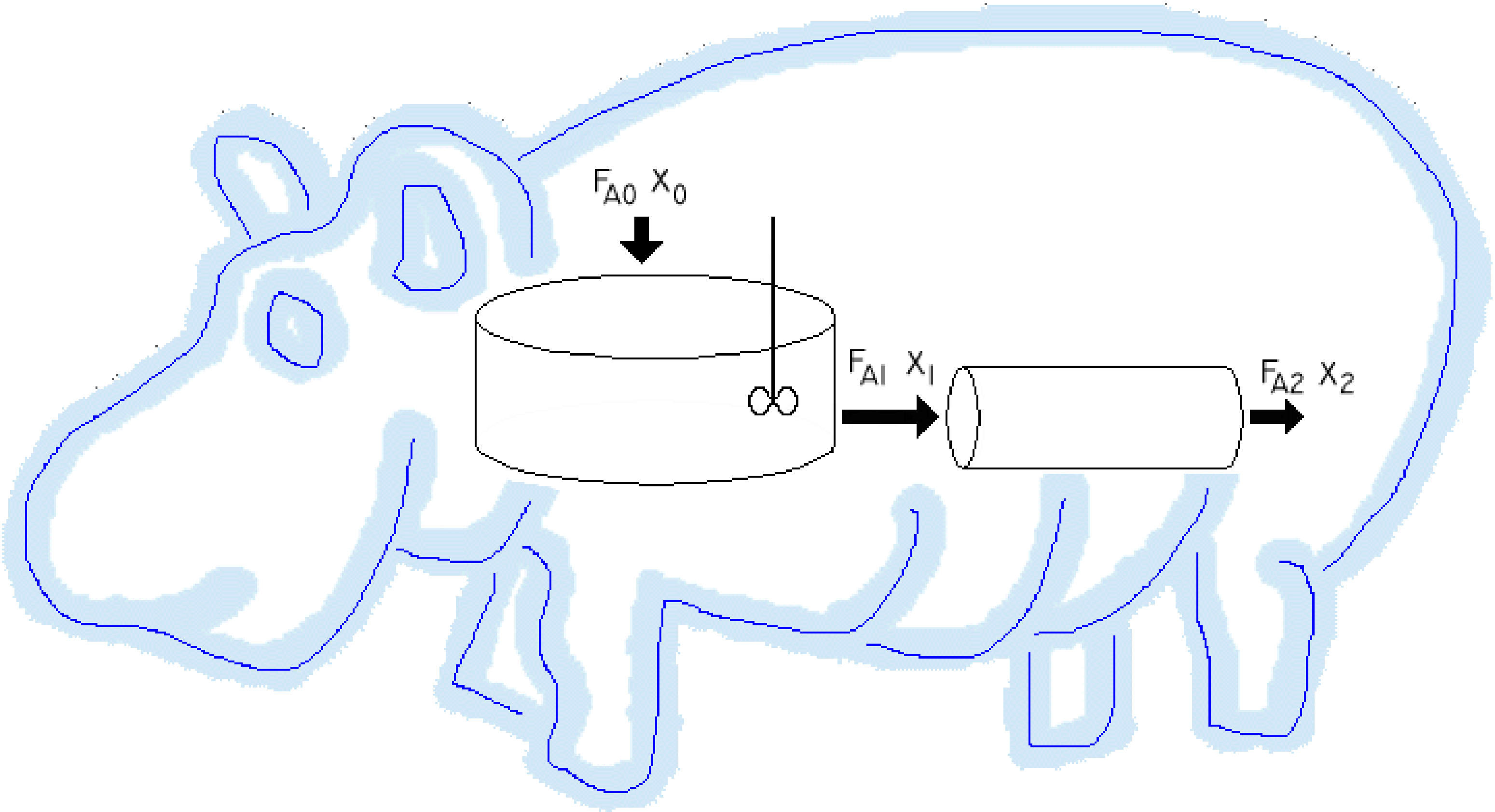
B) Batch

C) PFR

D) PBR

Assume that the hippo has to eat non-stop, and that although its stomach does not have an impeller, it is well mixed.

Flow in and out continuously, well mixed, must be a CSTR!



http://umich.edu/~essen/html/web_mod/hippo/equation4.htm

CSTR first, then flows out of stomach to gastrointestinal tract (more like a plug flow reactor).

We will learn about reactors in “series” soon!

Working on a problem together.

Let’s model the reaction in the hippo’s stomach (CSTR) with the following reaction and rate law

$$Food \rightarrow Products$$

$$A \rightarrow B$$

$$r_B = -r_A = kC_A$$

Based on the CSTR mole balance equation, is the molar flow rate out ($F_A = F_{A,out}$) higher or lower than in ($F_{A0} = F_{A,in}$)? What about for F_B vs. F_{B0}?

$$F_{A0} - F_A + r_A V = 0$$

$$F_{A0} - F_A - kC_A V = 0$$

$$F_{A0} - F_A = kC_A V; F_{A0} > F_A$$

$$F_{B0} - F_B + r_B V = 0$$

$$F_{B0} - F_B + kC_A V = 0$$

$$F_{B0} - F_B = -kC_A V; F_{B0} < F_B$$

Lets work through an example with numbers.

$A \rightarrow B$ in a batch reactor

What time, t, is needed to reduce the # of moles from N_{A0} to $N_A = 0.1\ N_{A0}$?

Our rate law is $-r_A = kC_A$ and $k = 0.046\ \text{min}^{-1}$.

Volume is constant.

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

$$r_A V = -kC_A V = -k\frac{N_A}{\cancel{V}}\cancel{V}$$

$$dt = \frac{1}{-kN_A} dN_A$$

$$\int_0^t dt = \int_{N_{A0}}^{0.1N_{A0}} \frac{1}{-kN_A} dN_A$$

$$t = \frac{1}{-k}(\ln N_A)\Big|_{N_{A0}}^{0.1N_{A0}} = \frac{1}{-k}[\ln(0.1N_{A0}) - \ln(N_{A0})]$$

$$t = \frac{1}{-k}[\ln(0.1)] = \frac{\ln(10)}{k}$$

$$t = \frac{\ln(10)}{0.046\ min^{-1}} \approx 50\ min$$

Question for thought:

If the rate constant k was larger, would the time required be higher or lower?

Lower! Faster reaction rate, takes less time

As the reaction proceeds, amounts of reactants/products will change

$$aA + bB \rightarrow cC + dD$$

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

To make it easy to know how much of species A has been converted (e.g., how much poisonous CO is converted), we monitor the reaction progress using conversion (X).

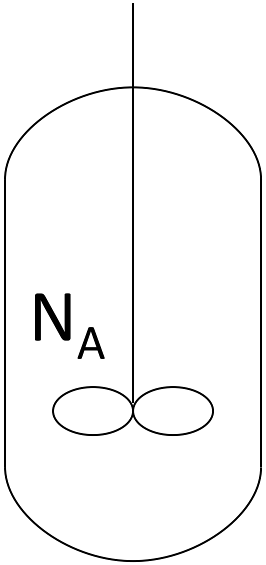
X ≡ moles A reacted / moles A fed

X = 0, no reaction has occurred

X = 1, the reaction has completed If A is limiting reactant

We cannot use conversion for multiple reactions or for reactors where mass is being removed or added, but it is very useful for designing reactors with a single reaction

Conversion in a batch reactor. Here moles A fed means the moles of A that were initially put into the reactor at time t=0. Recall in a batch reactor there is no flow in/out.



N_A N_{A0}

moles A remaining = moles A fed – moles A reacted

X ≡ moles A reacted / moles A fed

$N_A = N_{A0} - X\,N_{A0}$

$N_A = N_{A0}\,(1-X)$

$$X = \frac{N_{A0} - N_A}{N_{A0}}$$

Maximum conversion:

X = 1 for an irreversible reaction

X = X_{equil} for a reversible reaction

Design equation for a batch reactor using conversion.

We start with our batch design equation/mole balance on ‘A’

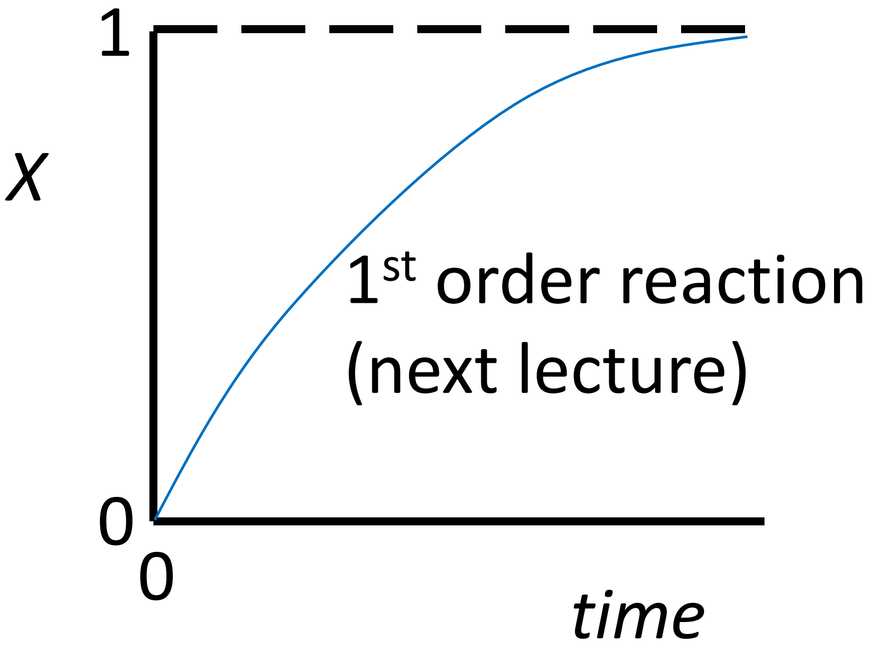
$$\frac{dN_A}{dt} = r_A V$$

$N_A = N_{A0}\,(1\text{-}X)$

$$\frac{d}{dt}\left(N_{A0}(1-X)\right) = -N_{A0}\frac{dX}{dt} = r_A V$$

$$\boxed{\frac{dX}{dt} = -\frac{r_A V}{N_{A0}}}$$

$$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$$



1st order reaction (next lecture)

Conversion in a flow reactor. (CSTR, PFR, PBR)

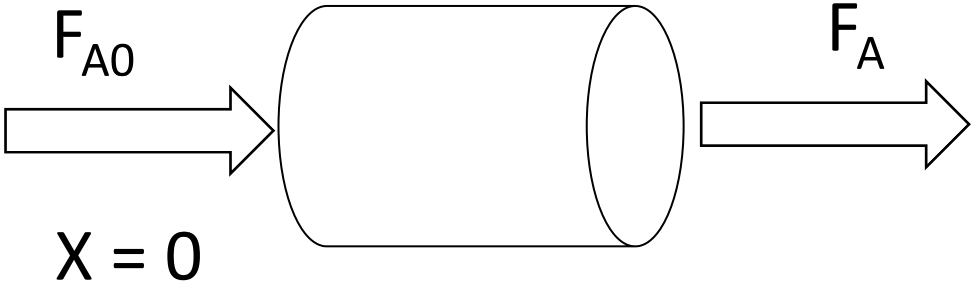
F_A F_{A0}

moles per time out = (moles/time) in – (moles/time) reacted

X ≡ moles A reacted / moles A fed

$F_A = F_{A0}\,(1\text{-}X)$

$$X = \frac{F_{A0} - F_A}{F_{A0}}$$



Molar flow rates and concentration

Liquids:

Assume constant volumetric flow rate, $v = v_0$

Gases:

$P_0V_0 = ZN_0RT_0$

$PV = ZNRT$

Z = compressibility factor, 1 for ideal gases

Volume

$$V = V_0 \frac{N}{N_0} \frac{T}{T_0} \frac{P_0}{P}$$

Volumetric flow rate

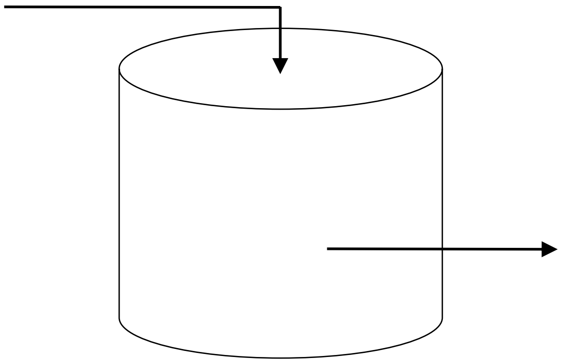
$$v = v_0 \frac{N}{N_0} \frac{T}{T_0} \frac{P_0}{P}$$

$$C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0}P_0}{RT_0} \qquad y_{A0} \equiv \frac{P_{A0}}{P_0}$$

For N we need stoichiometry (Lecture 4)

Design equation for a CSTR using conversion.

How large does my liquid-phase CSTR have to be to reach a given conversion?



$$v_0 = 10\ L/min$$

$$C_{A0}$$

$$F_{A0} = v_0 C_{A0}$$

$$v = v_0 = 10\ L/min$$

$$C_A = 0.1 C_{A0}$$

$$F_A = v C_A$$

$$V = \frac{F_A - F_{A0}}{r_A}$$

$$F_A = F_{A0}(1 - X)$$

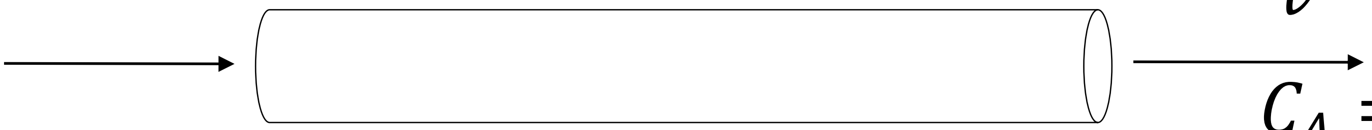
X = 0.9 (90%)

$$V = \frac{(F_{A0}(1 - X)) - F_{A0}}{r_A}$$

$$\boxed{V_{CSTR} = \frac{F_{A0} X}{-r_A}}$$

Design equation for a PFR using conversion.

How large does my PFR need to be to reach 80% conversion?



v_0

C_{A0}

$F_{A0} = v_0 C_{A0}$

v

$C_A = 0.2C_{A0}$

$F_A = vC_A$

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

$$F_A = F_{A0}(1 - X)$$

$$\frac{d(F_{A0}(1 - X))}{dV} = r_A$$

$$\int -F_{A0}dX = \int r_A dV$$

$$\int_0^X \frac{-F_{A0}}{r_A} dX = \int_0^{V_{PFR}} dV$$

$$\boxed{V_{PFR} = F_{A0} \int_0^X \frac{dX}{-r_A}}$$

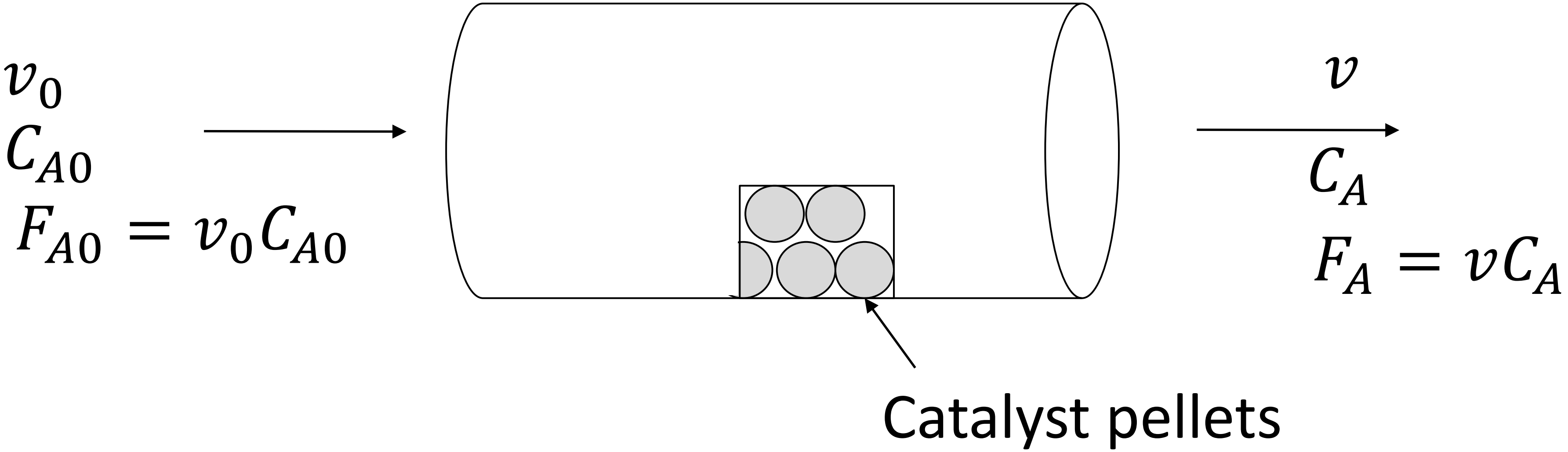
Design equation for a PBR using conversion.

How large does my PBR need to be to reach 80% conversion?

Same as PFR, just swap catalyst weight (W) for reactor volume and r_A' for r_A

$$\boxed{-r_A' = F_{A0}\frac{dX}{dW}}$$

$$\boxed{W_{PBR} = F_{A0}\int_0^X \frac{dX}{-r_A'}}$$



v_0

C_{A0}

$F_{A0} = v_0 C_{A0}$

v

C_A

$F_A = v C_A$

Catalyst pellets

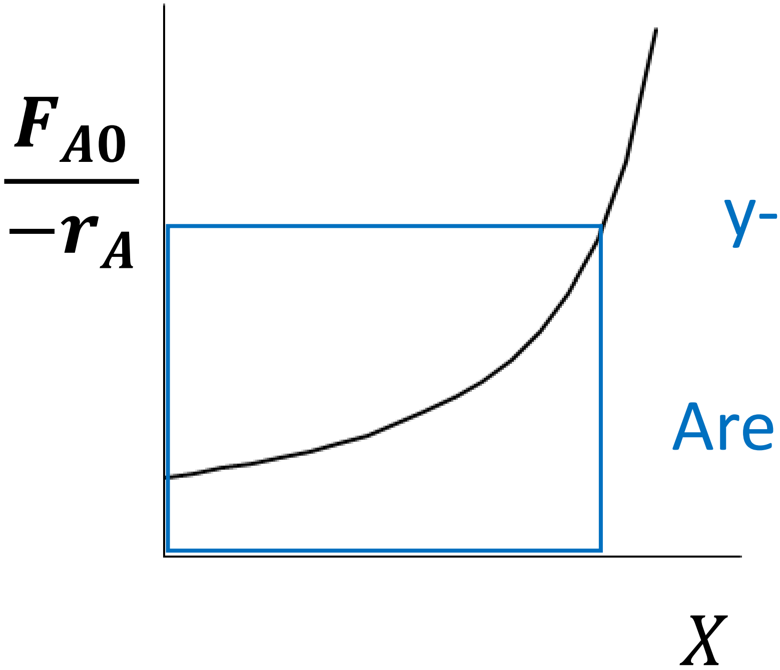
Generalized Mole Balance Equation in Conversion

Reactor	Differential	Algebraic	Integral
Batch	$N_{A0}\frac{dX}{dt} = -r_A V$		$t = N_{A0}\int_0^X \frac{dX}{-r_A V}$
CSTR		$V_{CSTR} = \frac{F_{A0}X}{-r_A}$	
PFR	$F_{A0}\frac{dX}{dV} = -r_A$		$V_{PFR} = F_{A0}\int_0^X \frac{dX}{-r_A}$
PBR	$-r_A' = F_{A0}\frac{dX}{dW}$		$W_{PBR} = F_{A0}\int_0^X \frac{dX}{-r_A'}$

Levenspiel plots for reactor sizing

- To size flow reactors, going to plot F_{A0}/-r_A vs. X

$$V_{CSTR} = \frac{\boldsymbol{F_{A0}}}{\boldsymbol{-r_A}} X \qquad V_{PFR} = \int_0^X \frac{\boldsymbol{F_{A0}}}{\boldsymbol{-r_A}} dX$$



y-axis * x-axis = V_{CSTR}

Area under curve = V_{PFR}

<u>Levenspiel</u> plots for reactor sizing example

Example: A → B, assume rate coefficient k, first order reaction, flow reactor

C_A raised to the power 1

$$r_A = -kC_A$$

Assuming isothermal and no pressure drop in reactor:

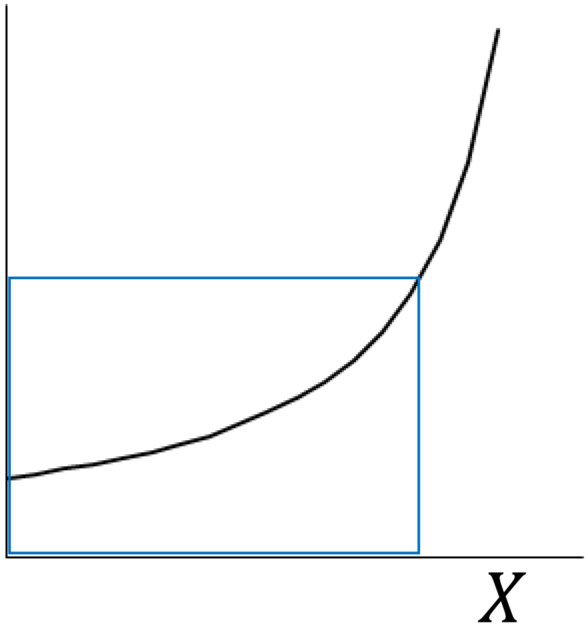
$$r_A = -kC_{A0}(1-X)$$

$$\frac{F_{A0}}{-r_A} = \frac{C_{A0}v_0}{-r_A} = \frac{\cancel{C_{A0}}v_0}{k\cancel{C_{A0}}(1-X)}$$

$$\frac{F_{A0}}{-r_A} = \frac{v_0}{k(1-X)}$$

$$V_{PFR} = \int_0^X \frac{-F_{A0}}{r_A} dX$$

$$\frac{F_{A0}}{-r_A} = \frac{v_0}{k(1-X)}$$

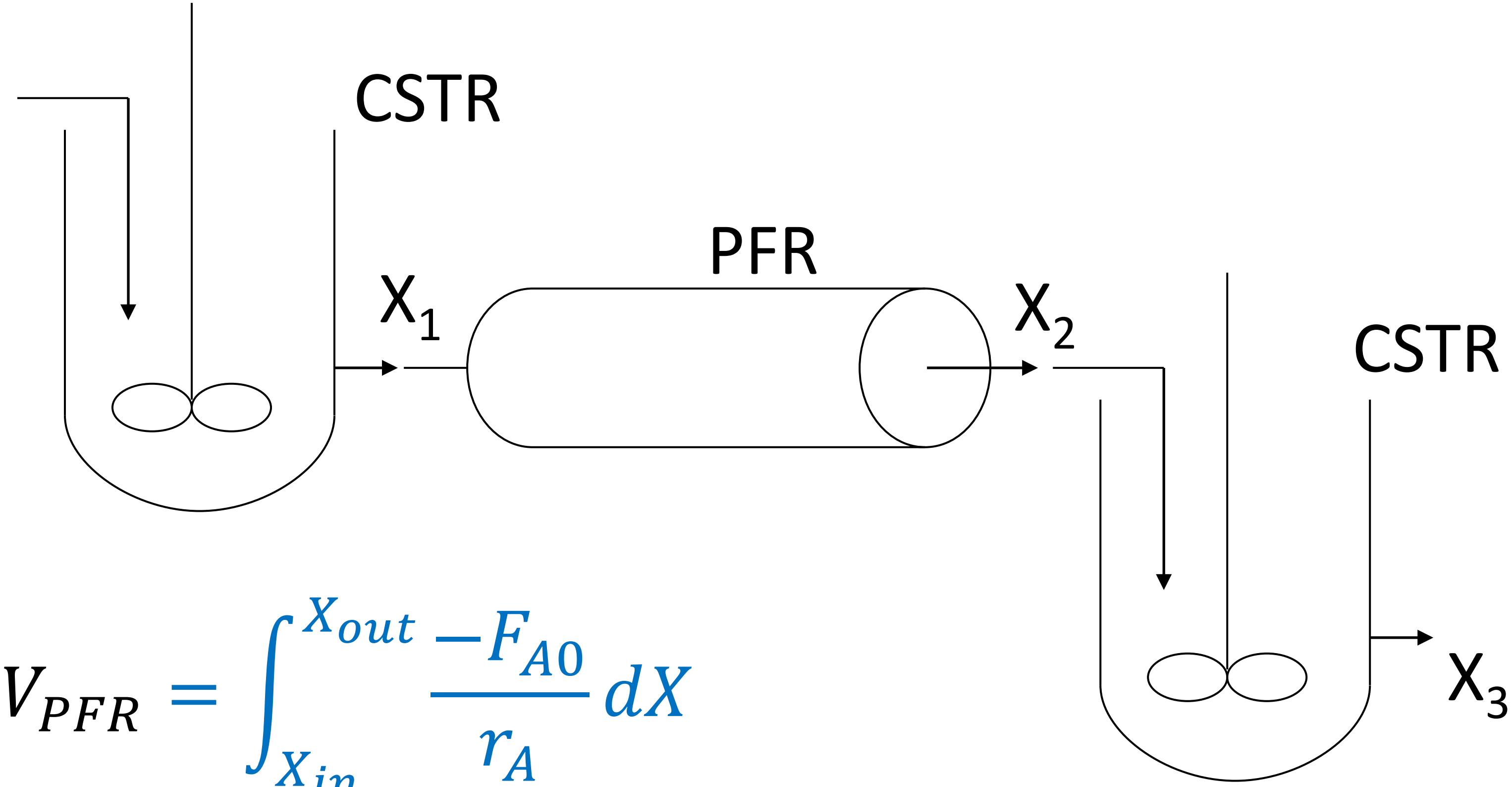


$$V_{CSTR} = \frac{F_{A0}X}{-r_A}$$

Tells us, for isothermal, no pressure drop case above:

If reaction order > 0, PFR will give lower volume than CSTR (area under curve smaller than rectangle)

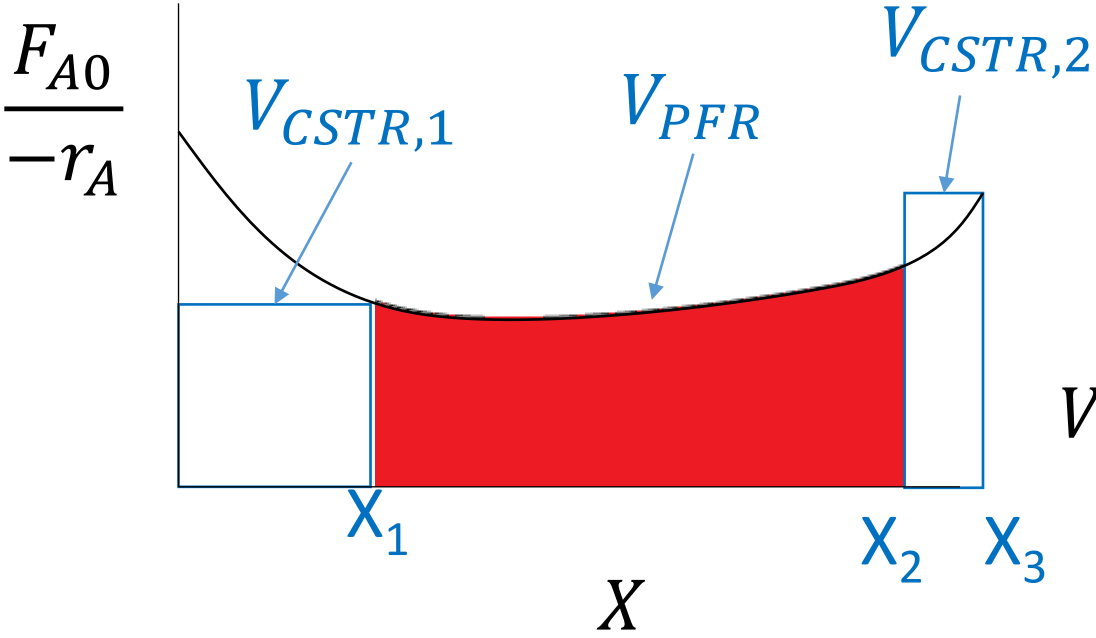
Reactors in series: Outlet of one reactor goes to inlet of another.



$$V_{PFR} = \int_{X_{in}}^{X_{out}} \frac{-F_{A0}}{r_A} dX$$

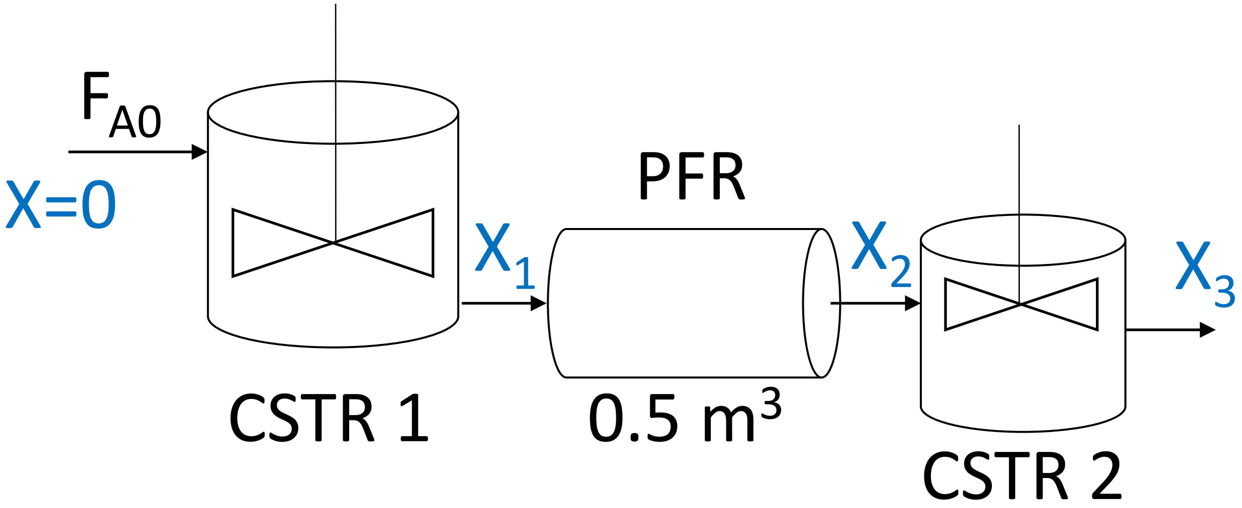
$$V_{CSTR} = \frac{F_{A0}(X_{out} - X_{in})}{-r_A}$$

Levenspiel for reactors in series



$$V_{PFR} = \int_{X_{in}}^{X_{out}} \frac{-F_{A0}}{r_A} dX$$

$$V_{CSTR} = \frac{F_{A0}(X_{out} - X_{in})}{-r_A}$$



To determine the integral for a PFR can approximate through various numerical methods (e.g. Simpson's one-third rule)

$$V = \int_0^X \frac{F_{A0}}{-r_A} dX \approx \frac{X/2}{3} F_{A0} \left[\frac{1}{-r_A(0)} + \frac{4}{-r_A(X/2)} + \frac{1}{-r_A(X)} \right]$$