Lecture 2

Chemical Reaction Engineering (CRE) is the field that studies the rates and mechanisms of chemical reactions and the design of the reactors in which they take place.

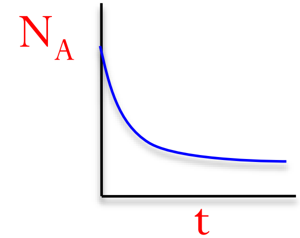
Lecture 2 – Tuesday

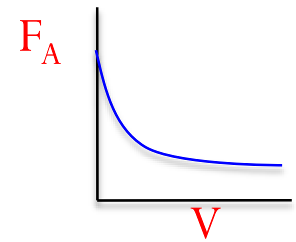
- Review of Lecture 1
- Definition of Conversion, X
- Develop the Design Equations in terms of X
- Size CSTRs and PFRs given $-r_A = f(X)$
- Conversion for Reactors in Series
- Review the Fall of the Tower of CRE

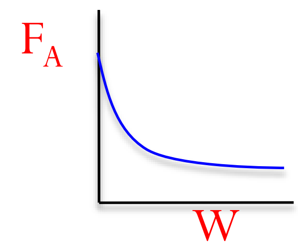
Reactor Mole Balances Summary

The GMBE applied to the four major reactor types (and the general reaction A→B)

Reactor	Differential	Algebraic	Integral
Batch	$\frac{dN_A}{dt} = r_A V$		$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$
CSTR		$V = \frac{F_{A0} - F_A}{-r_A}$	
PFR	$\frac{dF_A}{dV} = r_A$		$V = \int_{F_{A0}}^{F_A} \frac{dF_A}{dr_A}$
PBR	$\frac{dF_A}{dW} = r'_A$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$







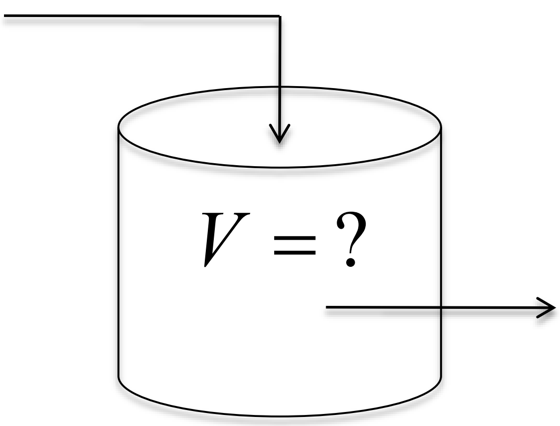
CSTR – Example Problem

Given the following information, Find V

$$\upsilon_0 = 10 \ \mathrm{dm^3}/\mathrm{min}$$

$$C_{A0}$$

$$F_{A0} = \upsilon_0 C_{A0}$$



$$\upsilon = \upsilon_0 = 10 \ \mathrm{dm^3}/\mathrm{min}$$

$$C_A = 0.1 C_{A0}$$

$$F_A = \upsilon C_A$$

Liquid phase

$$\upsilon = \upsilon_0$$

$$F_A = \upsilon_0 C_A$$

CSTR – Example Problem

(1) Mole Balance:

$$V = \frac{F_{A0} - F_A}{-r_A} = \frac{\upsilon_0 C_{A0} - \upsilon_0 C_A}{-r_A} = \frac{\upsilon_0 \left[C_{A0} - C_A\right]}{-r_A}$$

(2) Rate Law:

$$-r_A = kC_A$$

(3) Stoichiometry:

$$C_A = \frac{F_A}{\upsilon} = \frac{F_A}{\upsilon_0}$$

CSTR – Example Problem

(4) Combine:

$$V = \frac{\upsilon_0 \left[C_{A0} - C_A \right]}{k C_A}$$

(5) Evaluate:

$$C_A = 0.1 C_{A0}$$

$$V = \frac{\dfrac{10 dm^3}{\min} \left[C_{A0} - 0.1 C_{A0} \right]}{\left(0.23 \min^{-1}\right)\left(0.1 C_{A0}\right)} = \frac{10[1 - 0.1]}{(0.23)(0.1)} dm^3$$

$$\boxed{V = \frac{900}{2.3} = 391 dm^3}$$

Define conversion, X

Consider the generic reaction:

$$a\,A + b\,B \longrightarrow c\,C + d\,D$$

Chose limiting reactant A as basis of calculation:

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

Define conversion, X

$$X = \frac{\text{moles A reacted}}{\text{moles A fed}}$$

Batch

$$\begin{bmatrix} Moles\ A \\ remaining \end{bmatrix} = \begin{bmatrix} Moles\ A \\ initially \end{bmatrix} - \begin{bmatrix} Moles\ A \\ reacted \end{bmatrix}$$

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

$$dN_A = 0 - N_{A0}dX$$

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

Batch

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

$$t = 0 \quad X = 0$$

$$t = t \quad X = X$$

Integrating,

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

The necessary *t* to achieve conversion X.

CSTR

Consider the generic reaction:

$$a\,A + b\,B \longrightarrow c\,C + d\,D$$

Chose limiting reactant A as basis of calculation:

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

Define conversion, X

$$X = \frac{\text{moles A reacted}}{\text{moles A fed}}$$

CSTR

Steady State

$$\frac{dN_A}{dt} = 0$$

Well Mixed

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

$$\int r_A dV = r_A V$$

CSTR

$$\begin{bmatrix} Moles\ A \\ leaving \end{bmatrix} = \begin{bmatrix} Moles\ A \\ entering \end{bmatrix} - \begin{bmatrix} Moles\ A \\ reacted \end{bmatrix}$$

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

$$F_{A0} - F_A + \int r_A dV = 0$$

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

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

CSTR volume necessary to achieve conversion X.

PFR

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

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

Steady State $$dF_A = 0 - F_{A0}X$$

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

PFR

$$V = 0 \quad X = 0$$

$$V = V \quad X = X$$

Integrating,

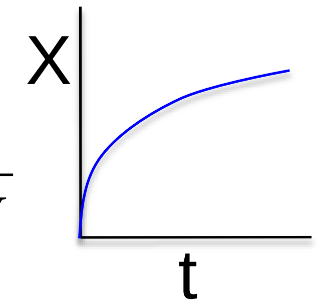
$$V = \int_0^X \frac{F_{A0}}{-r_A} dX$$

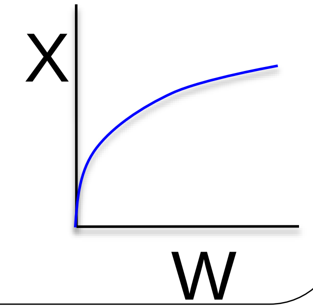
PFR volume necessary to achieve conversion X.

Reactor Mole Balances Summary

in terms of conversion, X

Reactor	Differential	Algebraic	Integral
Batch	$N_{A0}\dfrac{dX}{dt} = -r_A V$		$t = N_{A0}\displaystyle\int_0^X \dfrac{dX}{-r_A V}$
CSTR		$V = \dfrac{F_{A0}X}{-r_A}$	
PFR	$F_{A0}\dfrac{dX}{dV} = -r_A$		$V = \displaystyle\int_0^X \dfrac{F_{A0}dX}{-r_A}$
PBR	$F_{A0}\dfrac{dX}{dW} = -r'_A$		$W = \displaystyle\int_0^X \dfrac{F_{A0}dX}{-r'_A}$





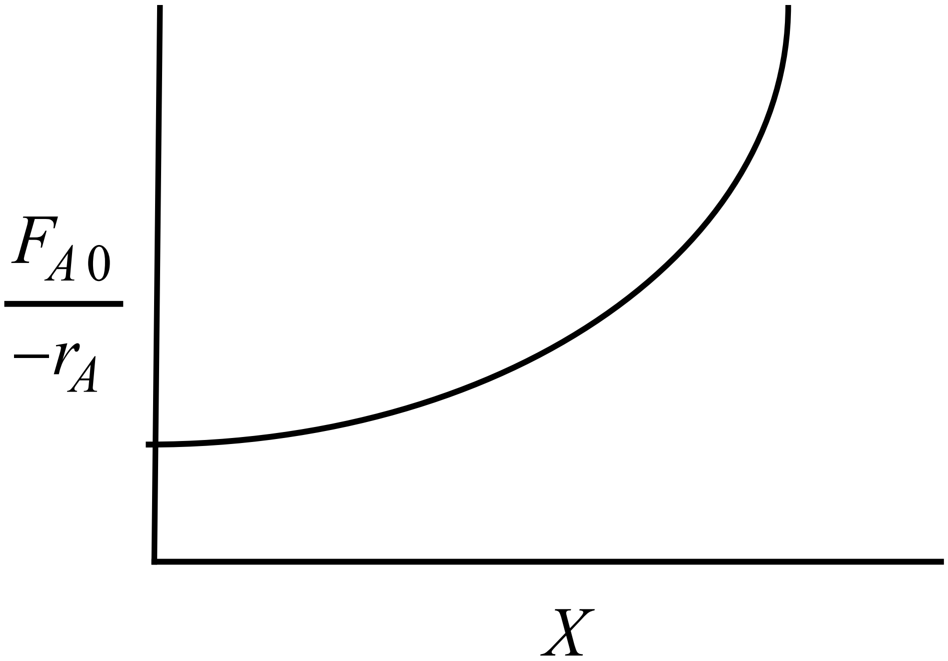
Levenspiel Plots

Reactor Sizing

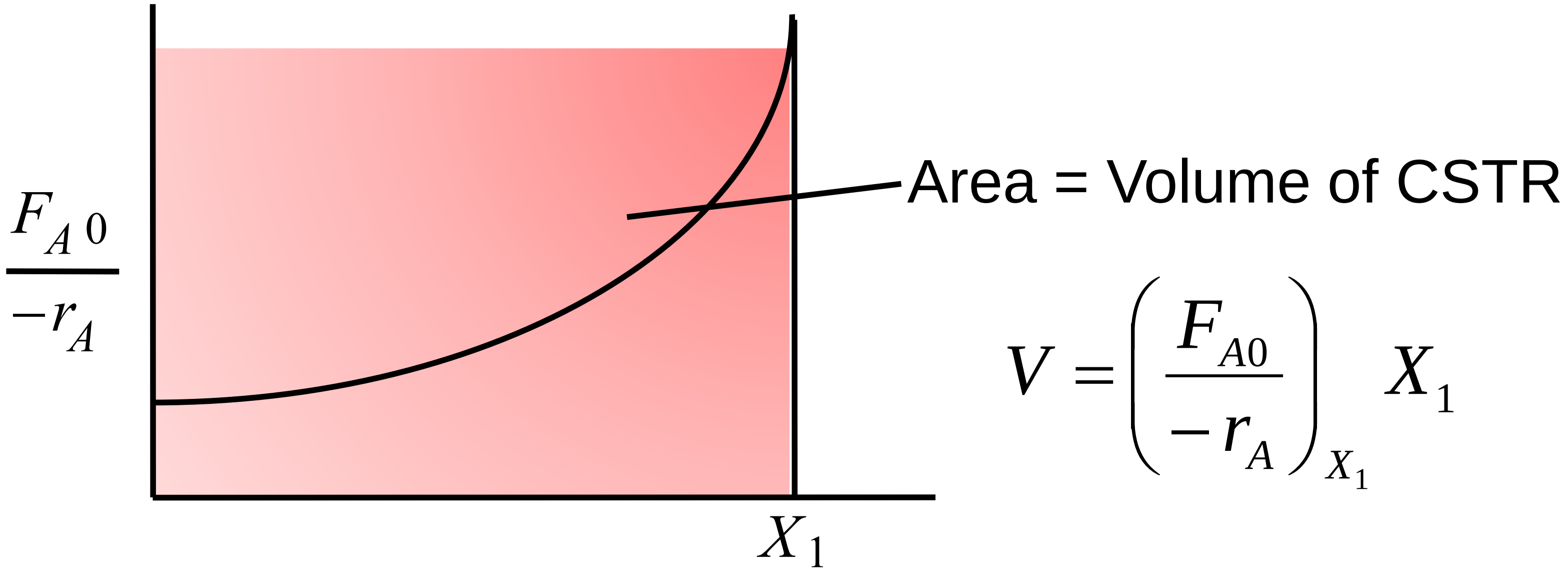
Given $-r_A$ as a function of conversion, **$-r_A = f(X)$,** one can size any type of reactor. We do this by constructing a Levenspiel plot. Here we plot either $(F_{A0}/-r_A)$ or $(1/-r_A)$ as a function of X. For $(F_{A0}/-r_A)$ vs. X, the volume of a CSTR and the volume of a PFR can be represented as the shaded areas in the Levenspiel Plots shown as:

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

Levenspiel Plots

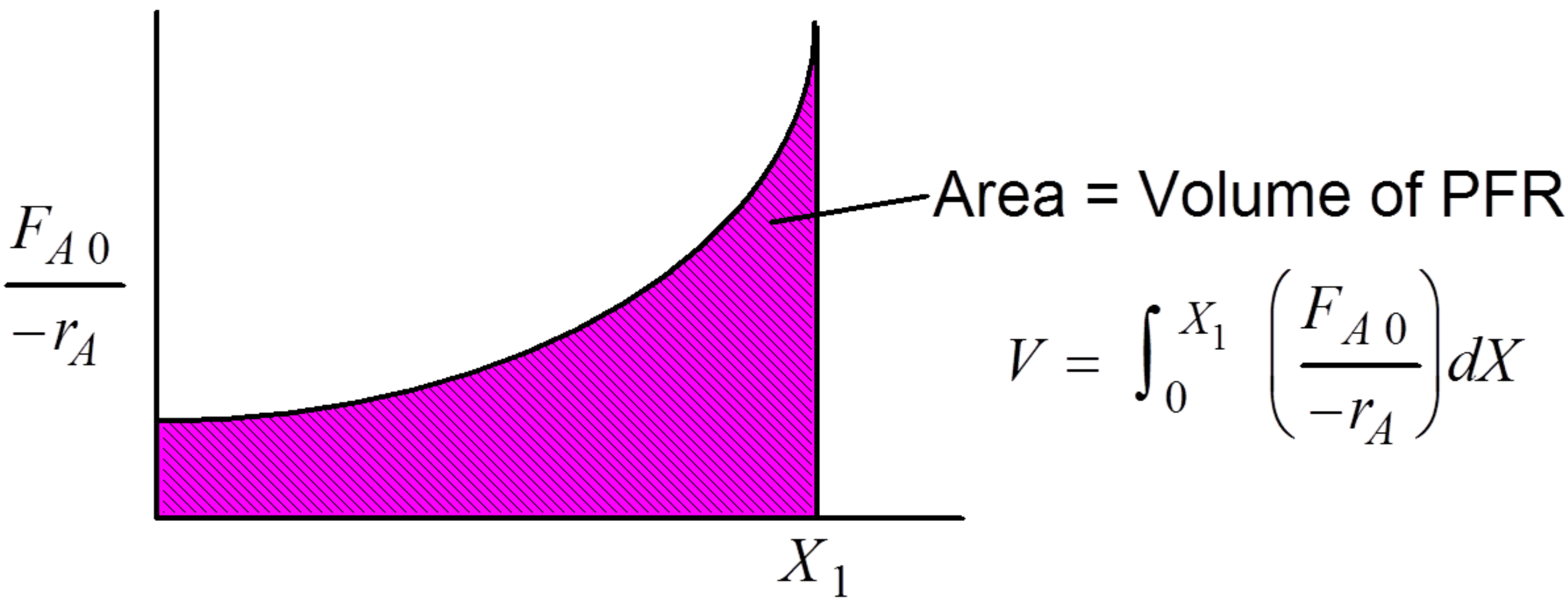


CSTR



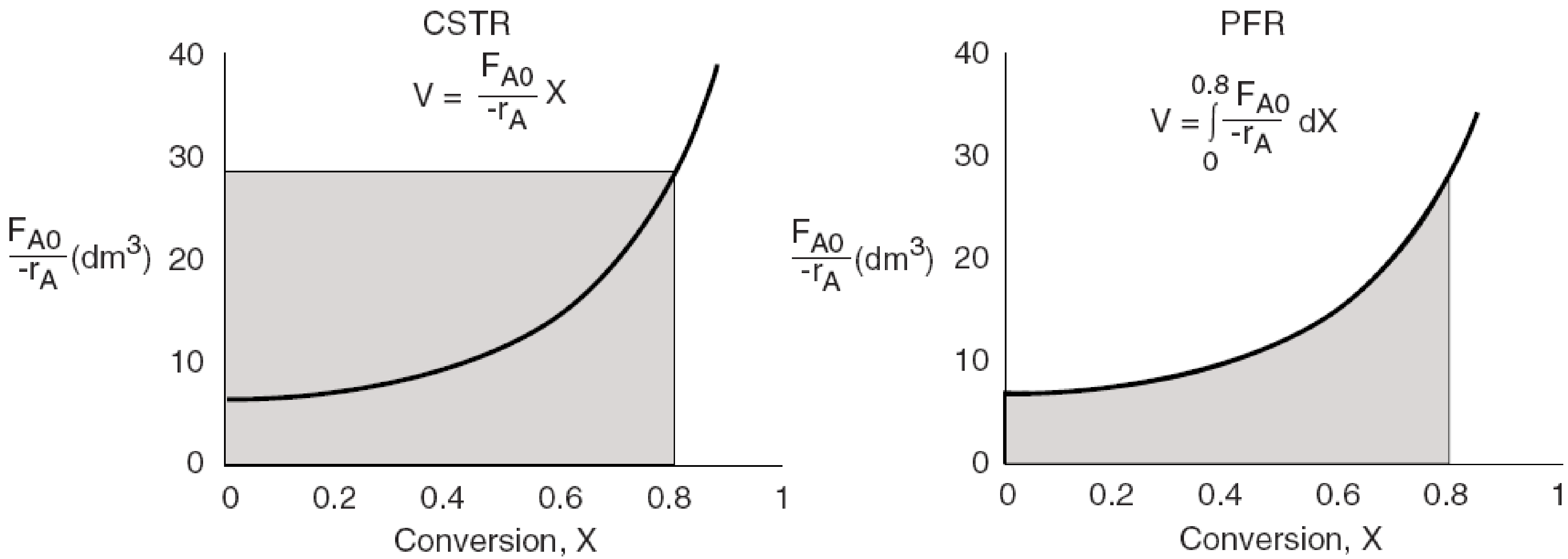
$$V = \left(\frac{F_{A0}}{-r_A}\right)_{X_1} X_1$$

PFR



$$V = \int_0^{X_1} \left(\frac{F_{A0}}{-r_A} \right) dX$$

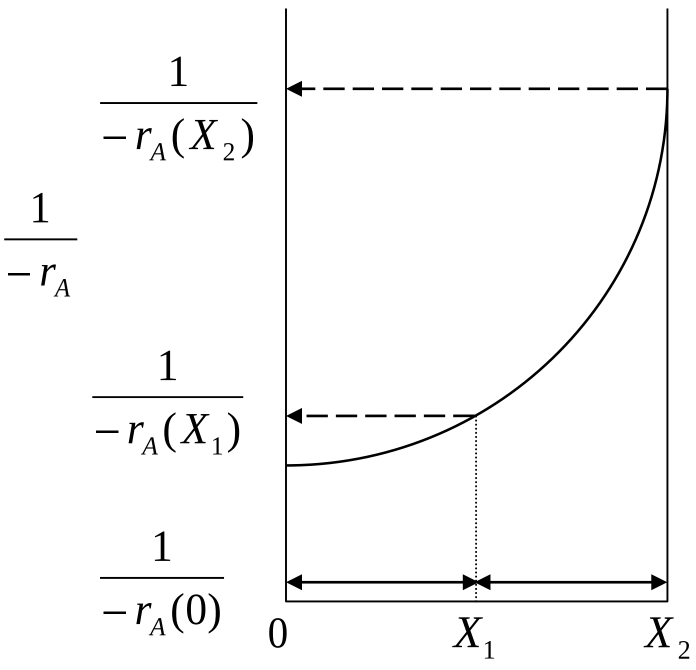
Levenspiel Plots



Numerical Evaluations of Integrals

- The integral to calculate the PFR volume can be evaluated using method as Simpson's One-Third Rule: (See Appendix A.4)

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



Other numerical methods are:

- Trapezoidal Rule (uses two data points)
- Simpson's Three-Eight's Rule (uses four data points)
- Five-Point Quadrature Formula

Reactors in Series

Given: r_A as a function of conversion, one can also design any sequence of reactors in series by defining X:

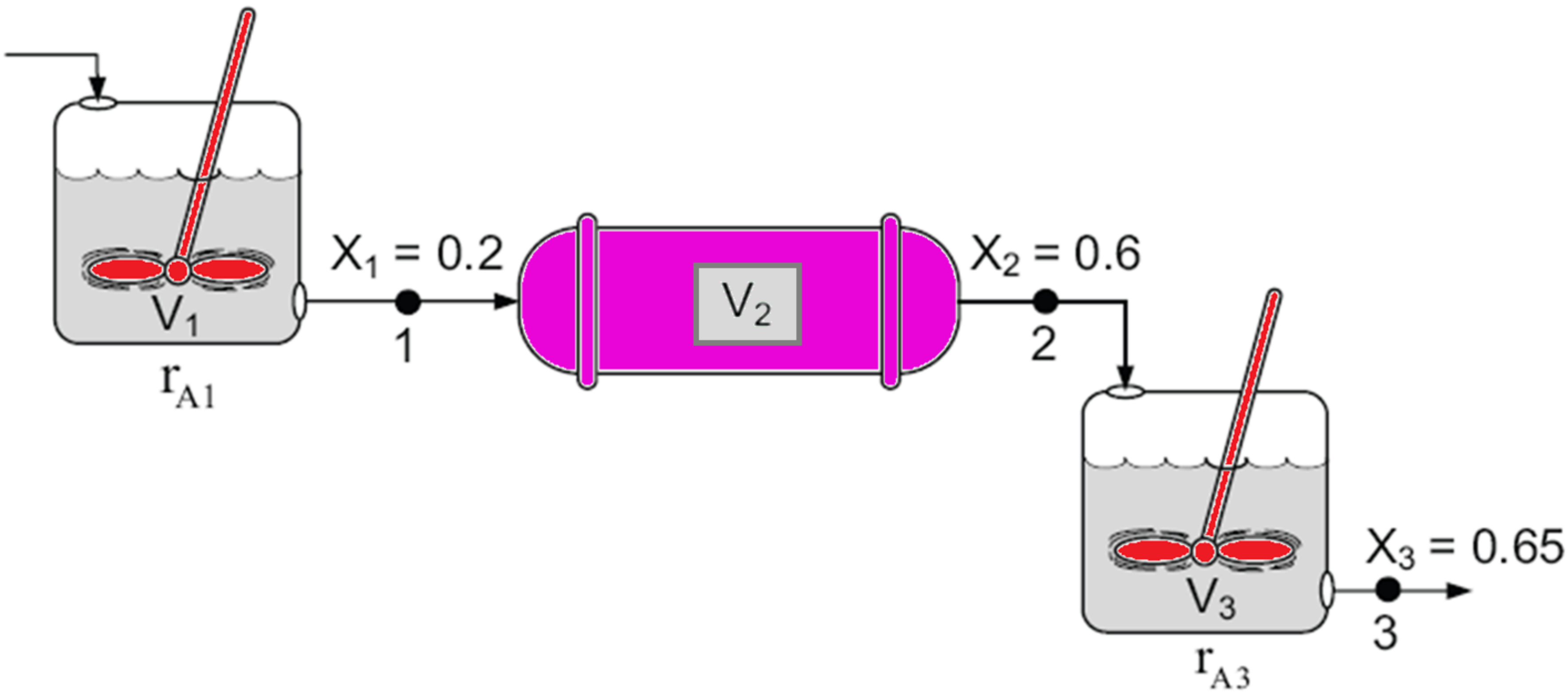
$$X_i = \frac{\text{total moles of A reacted up to point i}}{\text{moles of A fed to first reactor}}$$

Only valid if there are no side streams.

Molar Flow rate of species A at point i:

$$F_{Ai} = F_{A0} - F_{A0} X_i$$

Reactors in Series

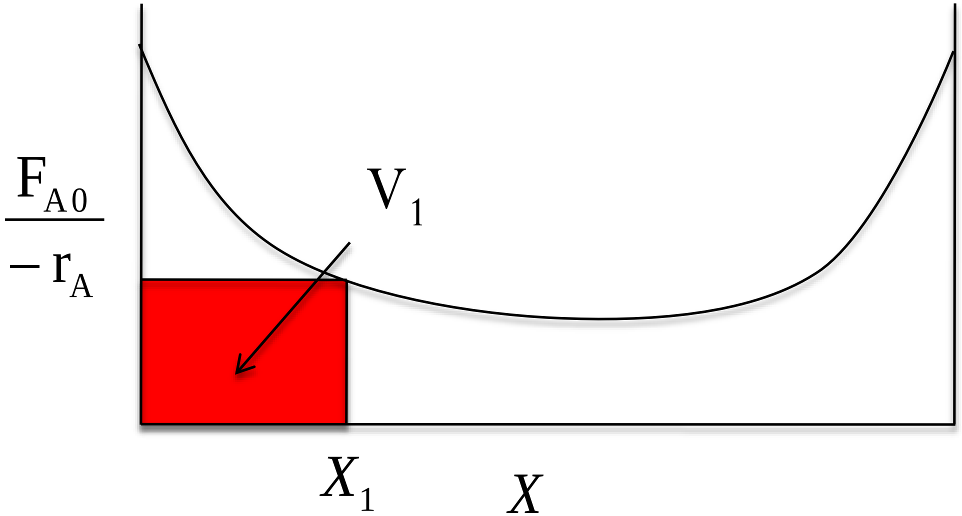


Reactors in Series

Reactor 1:

$$F_{A1} = F_{A0} - F_{A0}X_1$$

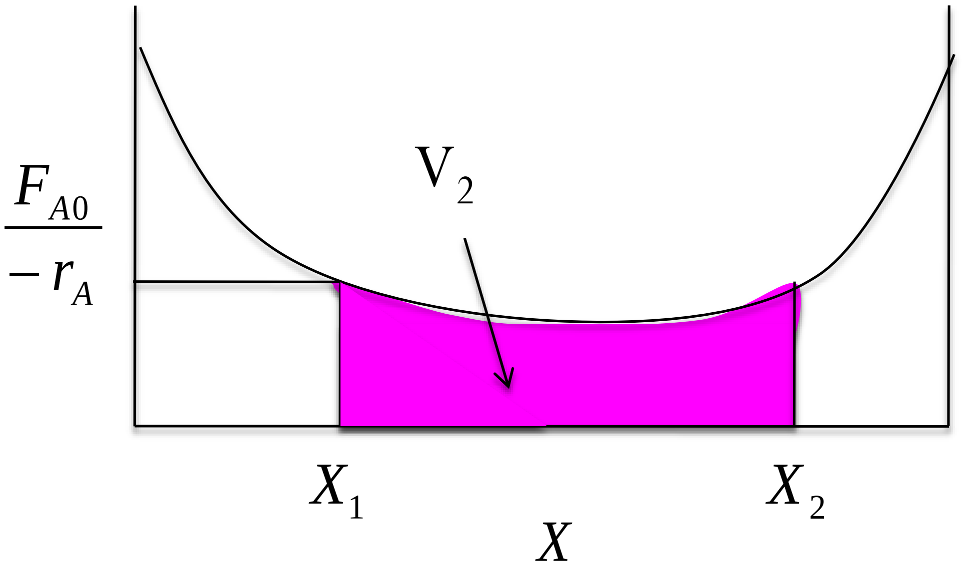
$$V_1 = \frac{F_{A0} - F_{A1}}{-r_{A1}} = \frac{F_{A0} - \left(F_{A0} - F_{A0}X_1\right)}{-r_{A1}} = \frac{F_{A0}X_1}{-r_{A1}}$$



Reactors in Series

Reactor 2:

$$V_2 = \int_{X_1}^{X_2} \frac{F_{A0}}{-r_A} dX$$



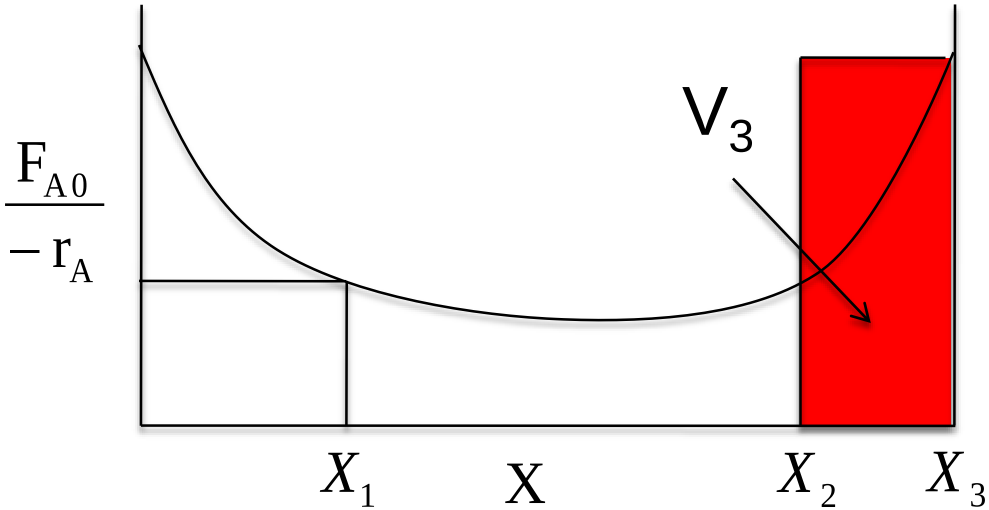
Reactors in Series

Reactor 3:

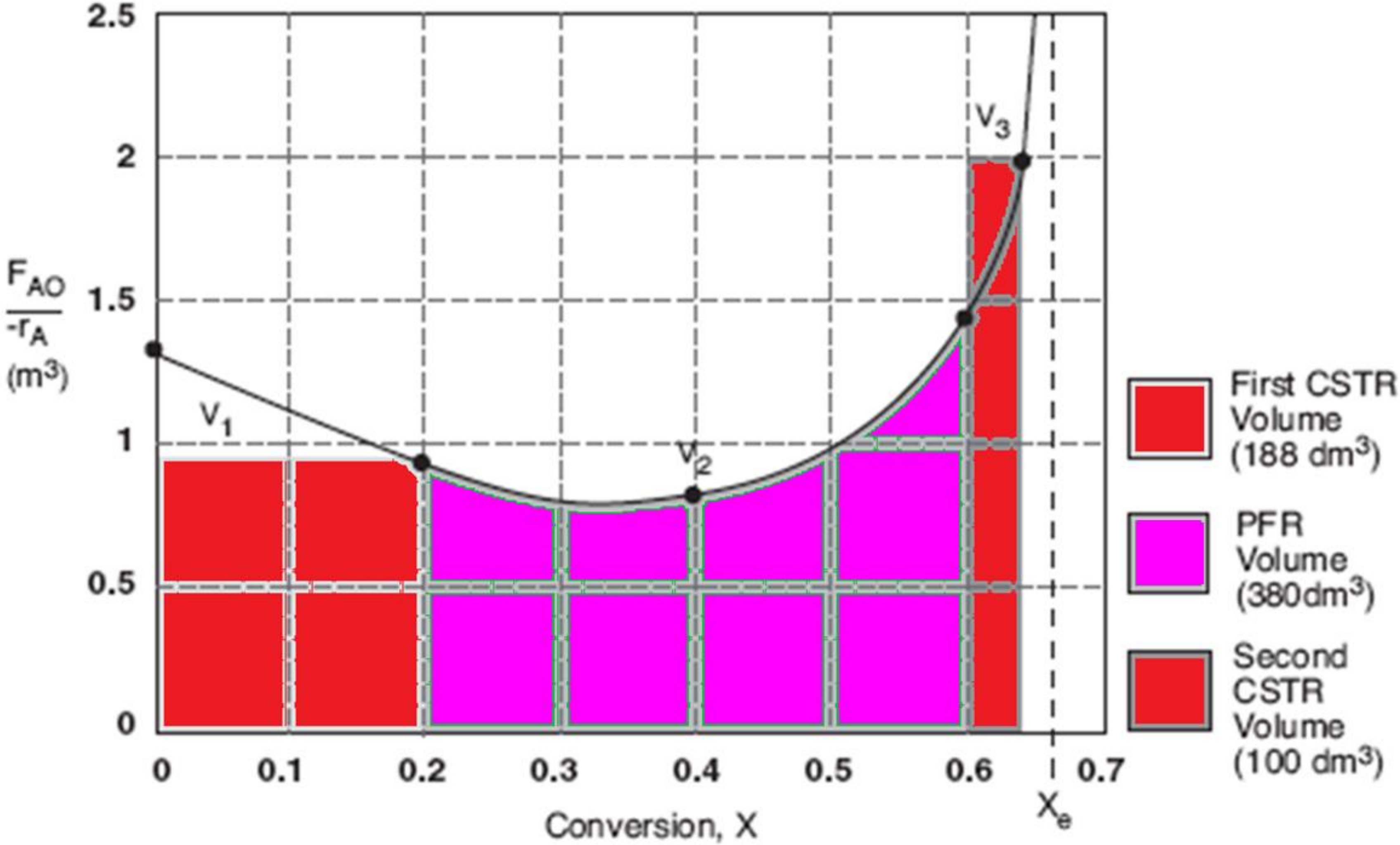
$$F_{A2} - F_{A3} + r_{A3}V_3 = 0$$

$$\left(F_{A0} - F_{A0}X_2\right) - \left(F_{A0} - F_{A0}X_3\right) + r_{A3}V_3 = 0$$

$$V_3 = \frac{F_{A0}\left(X_3 - X_2\right)}{-r_{A3}}$$



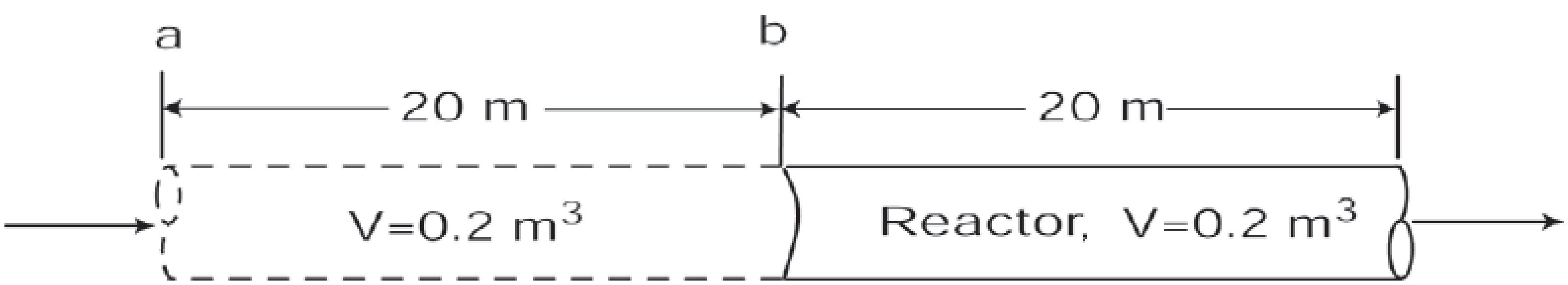
Reactors in Series



Reactors in Series

Space time τ is the time necessary to process 1 reactor volume of fluid at entrance conditions.

$$\tau = \frac{V}{\upsilon_0}$$



KEEPING UP

- The tower of CRE, is it stable?

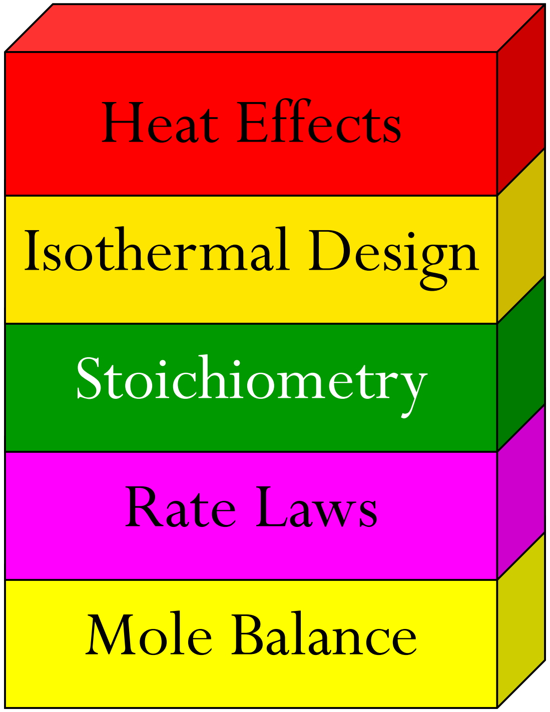
Reaction Engineering

Mole Balance

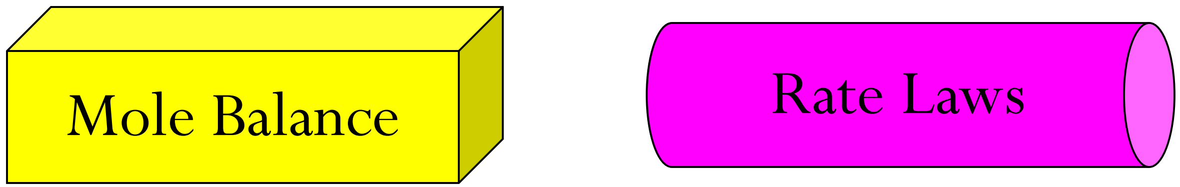
Rate Laws

Stoichiometry

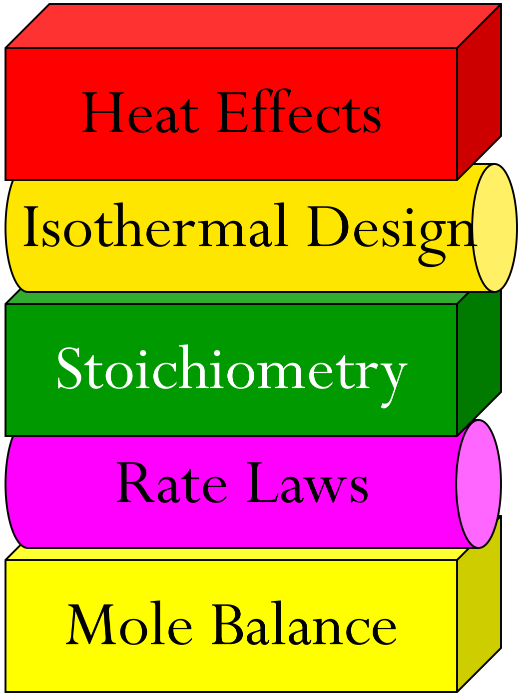
These topics build upon one another.



CRE Algorithm



Be careful not to cut corners on any of the **CRE building blocks** while learning this material!



Otherwise, your Algorithm becomes unstable.

End of Lecture 2