Chemical Reaction Engineering I

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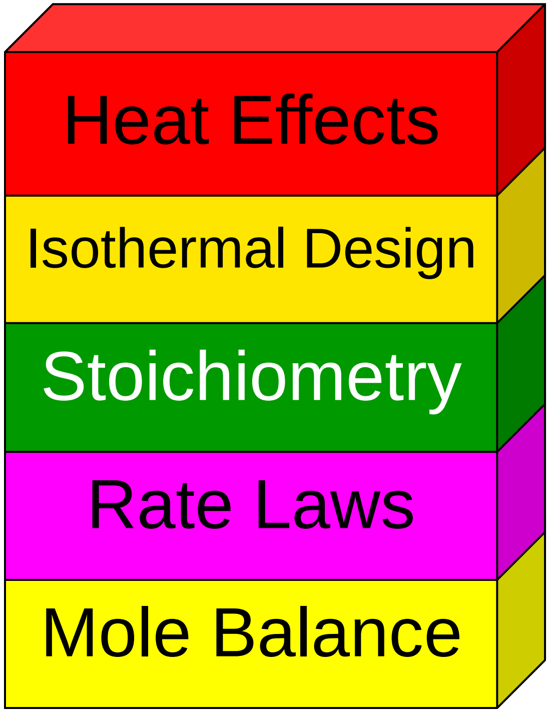
CHAPTER 2 – CONVERSION AND REACTOR SIZING

Be more concerned with your character than with your reputation, because character is what you really are, while reputation is merely what others think you are.

John Wooden, coach, UCLA Bruins

Learning Outcomes

- After completing Chapter 2, you should be able to:
  - Define conversion and space time.
  - Write the mole balances in terms of conversion for a batch reactor, CSTR, PFR, and PBR.
  - Size reactors either alone or in series once given the molar flow rate of A, and the rate of reaction, $-r_A$, as a function of conversion, X.



Heat Effects

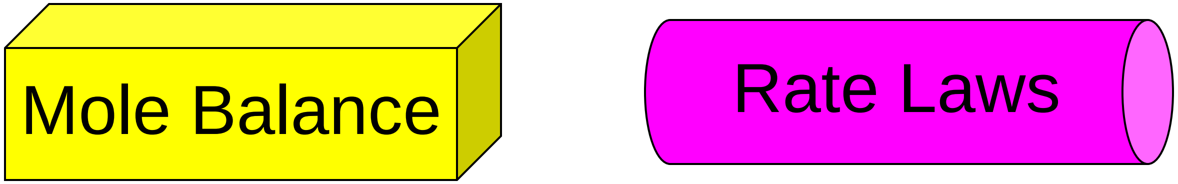
Isothermal Design

Stoichiometry

Rate Laws

Mole Balance

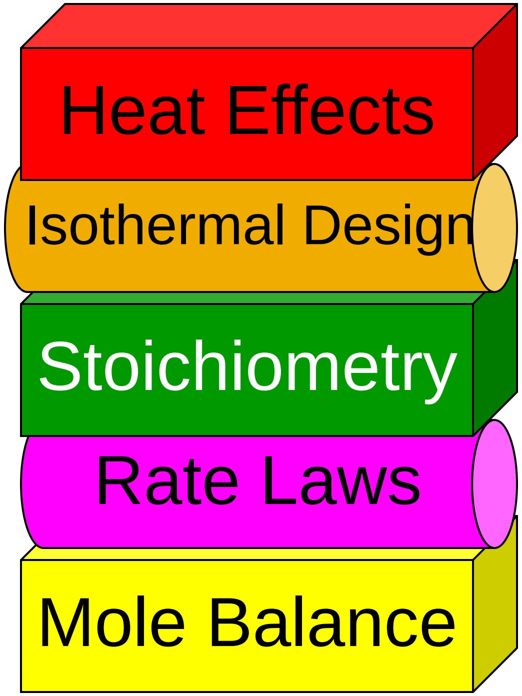
CRE Algorithm



Mole Balance

Rate Laws

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

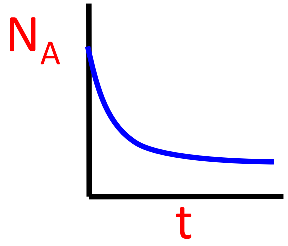
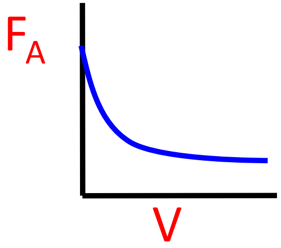
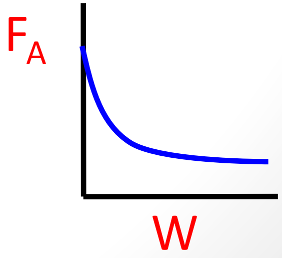


Otherwise, your Algorithm becomes unstable.

Review Chapter 1

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	$\frac{dF_A}{dW} = r'_A$		$W = \int_{F_{A0}}^{F_A} \frac{dF_A}{r'_A}$	

Definition of Conversion

- Consider the generic reaction:

$$aA + bB \longrightarrow cC + dD$$

- Choose **limiting reactant A as basis** of calculation:

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

- Define **conversion**, X_A: the number of moles of A that have reacted per mole of A fed to the system

$$X_A = \frac{moles\ A\ reacted}{moles\ A\ fed}$$

  - **For Batch System:** "Moles A fed" is the amount of A at the start of the reactor (at $t = 0$)
  - **For Flow System:** "Moles A fed" is the amount of A entering the reactor

Conversion Example

$$A + 2B \rightarrow 2C$$

- Start with 1 mole of A and 1 mole of B
- **What is the limiting reactant?**

Conversion Example

$$A + 2B \rightarrow 2C$$

- Start with 1 mole of A and 1 mole of B
- If A is the basis and at the end we have:

1 mole A, 1 mole B ↔ X_A = 0/1 = 0 (no reaction)

½ mole A, 0 mole B ↔ X_A = 0.5/1 = ½

0 mole A, -1 mole B ↔ X_A = 1/1 = 1 (complete reaction)

Not possible!

- The correct approach is to take B as the basis because <u>B is the limiting reagent</u>
- At the end we have:

1 mole A, 1 mole B ↔ X_B = 0/1 = 0 (no reaction)

½ mole A, 0 mole B ↔ X_B = 1/1 = 1 (complete reaction)

Expressing other Components Conversion in Terms of X_A

$$A + \frac{b}{a}B \longrightarrow \frac{c}{a}C + \frac{d}{a}D \qquad X_A \equiv \frac{\text{moles A reacted}}{\text{moles A fed}}$$

BATCH SYSTEM:

Longer reactant is in reactor, more reactant is converted to product (until reactant is consumed or the reaction reaches equilibrium)

∴ Conversion (X_j) is a function of time (t) in the batch reactor

$$N_A = N_{A0} - [N_{A0}][X_A]$$

Moles A in reactor at time t = Moles A fed - Moles A consumed

$$\rightarrow N_A = N_{A0}(1 - X_A)$$

reactant

product

$$N_B = N_{B0} - \frac{b}{a}(N_{A0}X_A) \qquad N_C = N_{C0} + \frac{c}{a}(N_{A0}X_A)$$

$$N_D = N_{D0} + \frac{d}{a}(N_{A0}X_A) \qquad N_I = N_{I0} \quad (\text{inert component})$$

Batch Reactor

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

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

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

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

Batch Reactor

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

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

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

Integrating,

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

The necessary t to achieve conversion X.

CSTR

Consider the generic reaction:

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

Choose 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

$$\int r_A dV = r_A V$$

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

CSTR

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

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

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

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

CSTR *volume* necessary to achieve conversion *X*.

PFR

Steady State

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

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

$$dF_A = 0 - F_{A0}dX$$

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

PFR

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

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

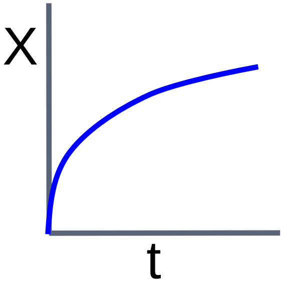
Integrating,

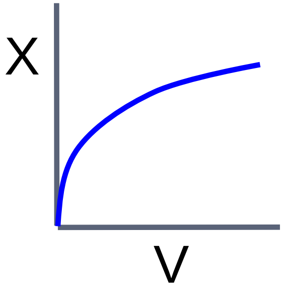
$$\boxed{V = \int_0^X \frac{F_{A0}}{-r_A} dX}$$

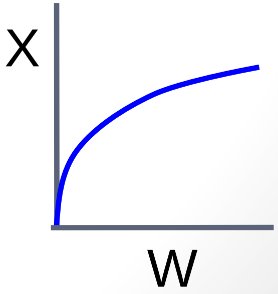
PFR *volume* necessary to achieve conversion *X*.

Reactor Mole Balances Summary in terms of conversion, X

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







Applications of the Design Equations for Continuous-Flow Reactors

Levenspiel Plots

Reactor Sizing

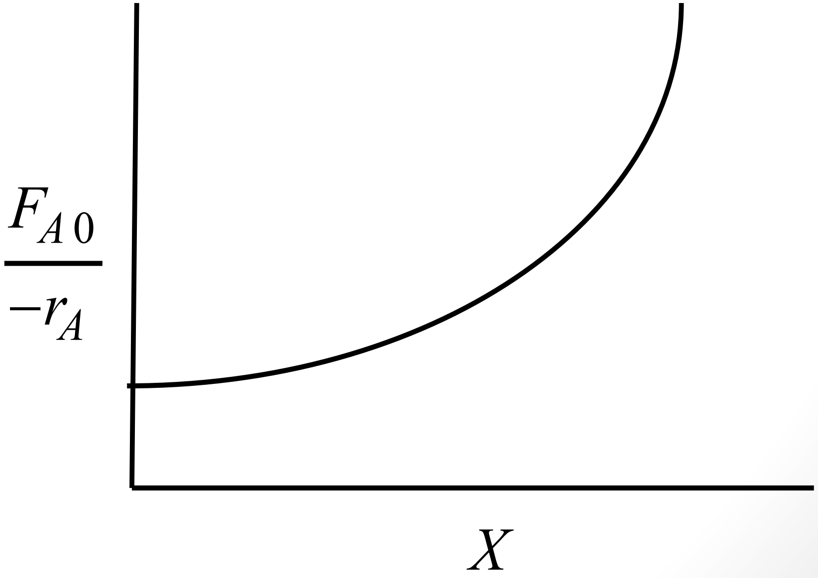
- Given $-r_A$ as a function of conversion, $-\boldsymbol{r_A} = \boldsymbol{f}(\boldsymbol{X})$**,** one can size any isothermal reaction system.
- We do this by constructing **Levenspiel plot**. Here we plot either $(F_{A0}/-r_A)$ or $(1/-r_A)$ as a function of X.
  - For $(F_{A0}/-r_A)$ vs. X, the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

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

Levenspiel Plots

- For all irreversible reactions of order > zero, as we approach complete conversion where all the limiting reactant is used up, i.e. $X = 1$, the reciprocal rate approaches infinity as does the reactor volume, i.e.

- As $X \rightarrow 1$, $-r_A \rightarrow 0$, thus $\frac{1}{-r_A} \rightarrow \infty$, therefore $V \rightarrow \infty$.



Levenspiel Plots

- For reversible reactions, the maximum conversion is the equilibrium conversion X_e.
- At equilibrium, the reaction rate is zero ($\boldsymbol{-r_A \equiv 0}$).

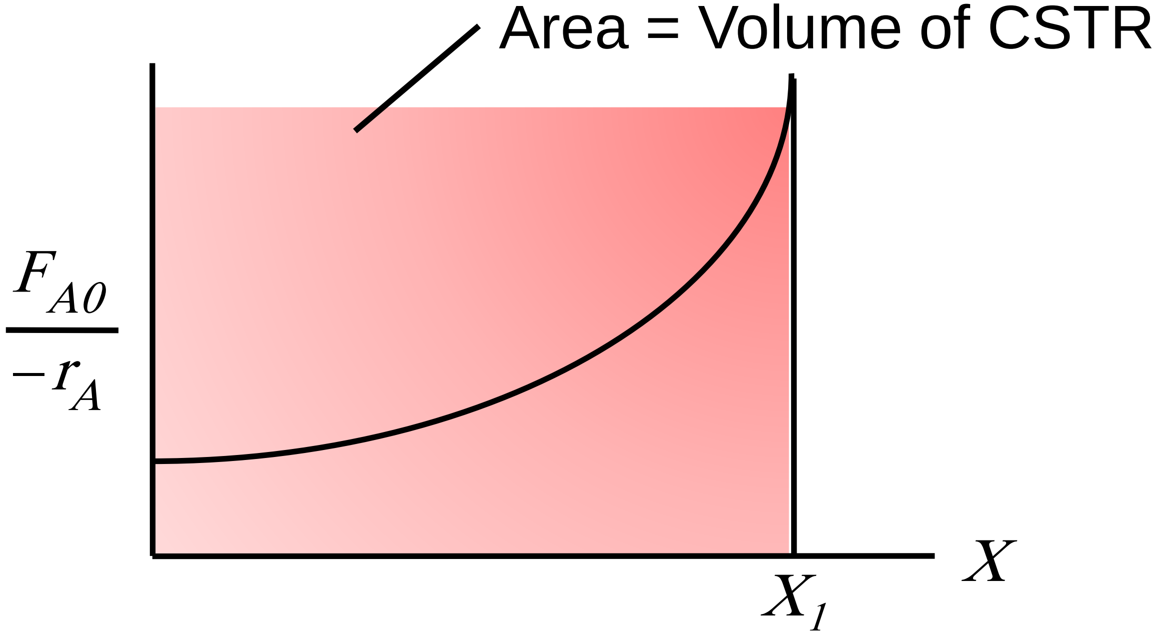
  Therefore:

  As $X \rightarrow X_e$, $-r_A \rightarrow 0$,

  thus $\frac{1}{-r_A} \rightarrow \infty$, and therefore $V \rightarrow \infty$.

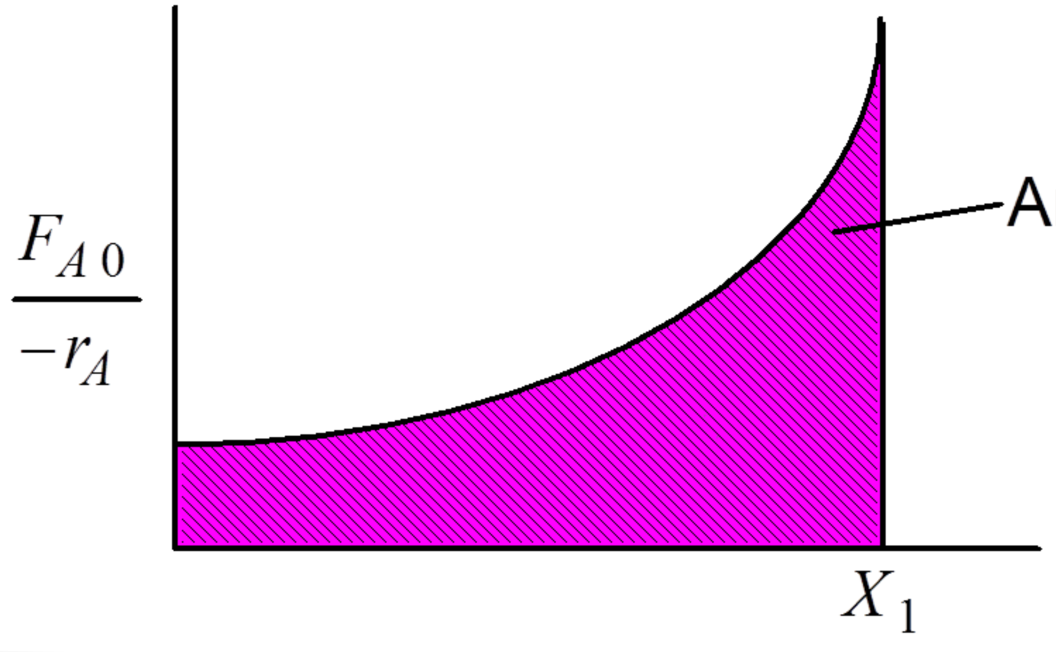
CSTR

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



PFR

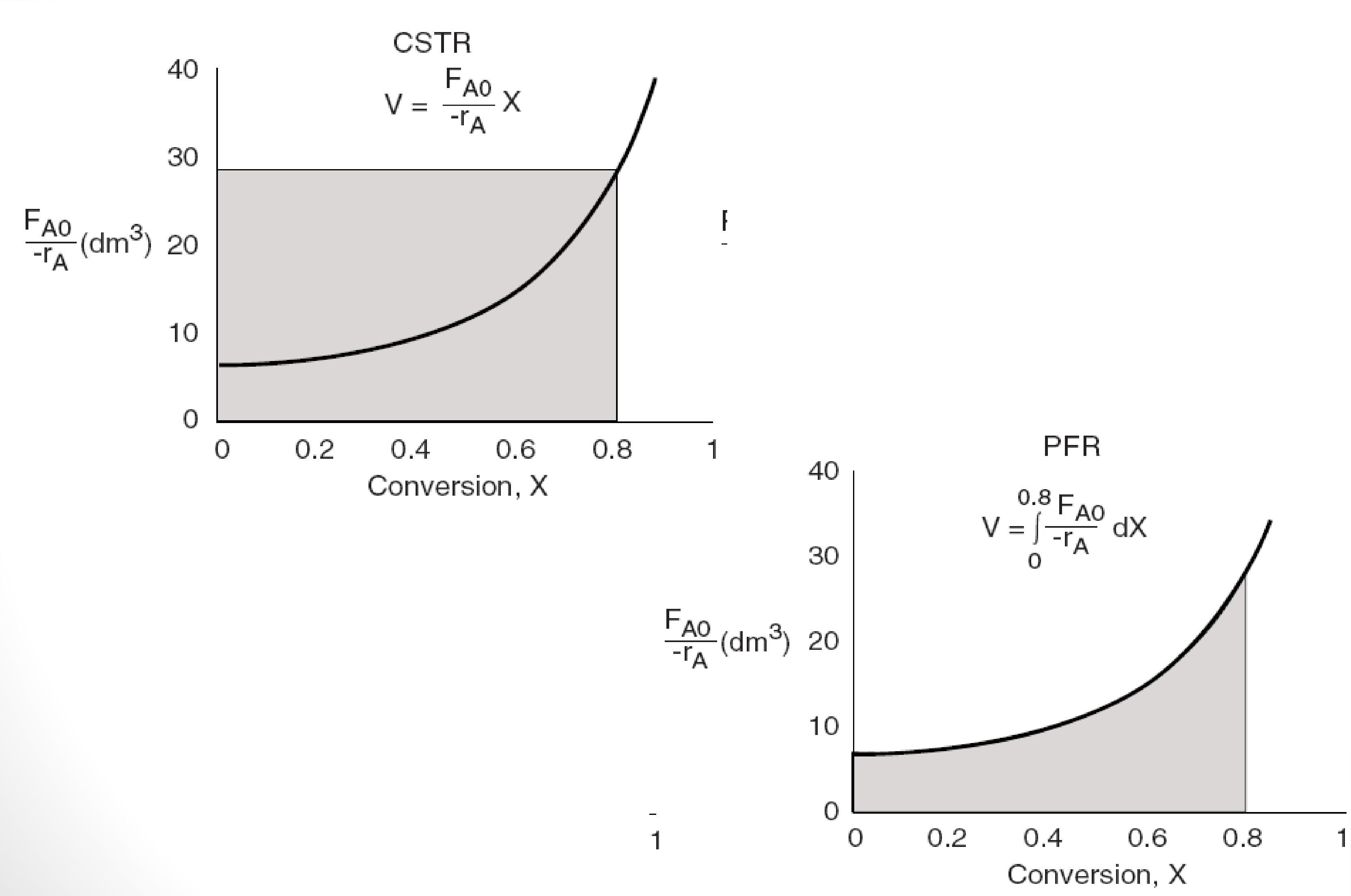
$$V = \int_0^X \frac{F_{A0}\,dX}{-r_A}$$



Area = Volume of PFR

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

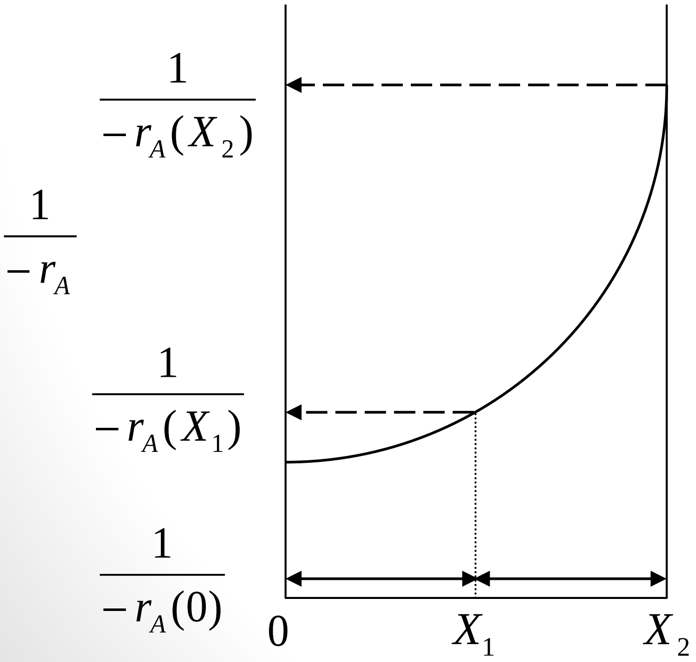
Levenspiel Plots



Numerical Evaluations of Integrals

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

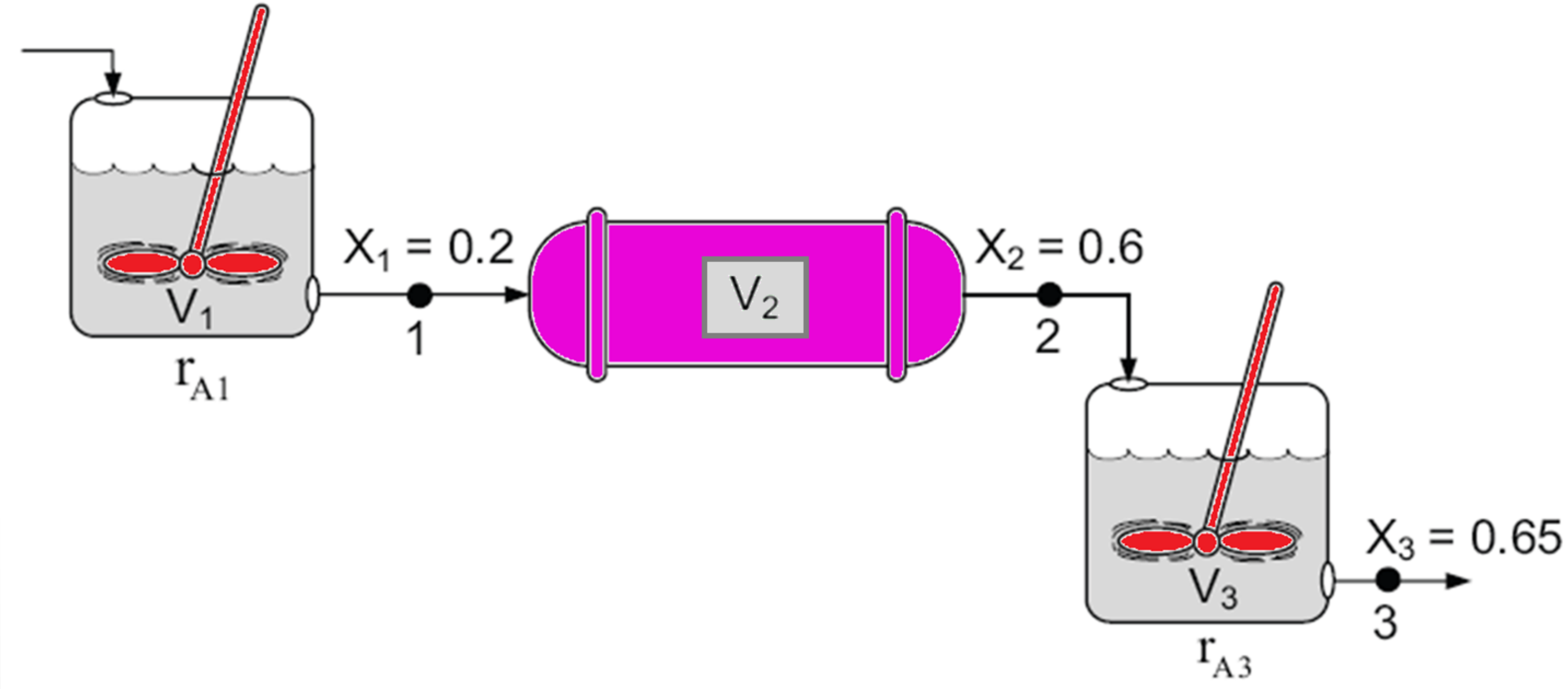
$$V = \int_0^X \frac{F_{A0}}{-r_A} dX = \frac{\Delta x}{3} F_{A0}\left[\frac{1}{-r_A(0)} + \frac{4}{-r_A(X/2)} + \frac{1}{-r_A(X)}\right]$$



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



Reactors in Series

- Given: $-rA$ as a function of conversion, one can also design any sequence of reactors in series by defining X_i:

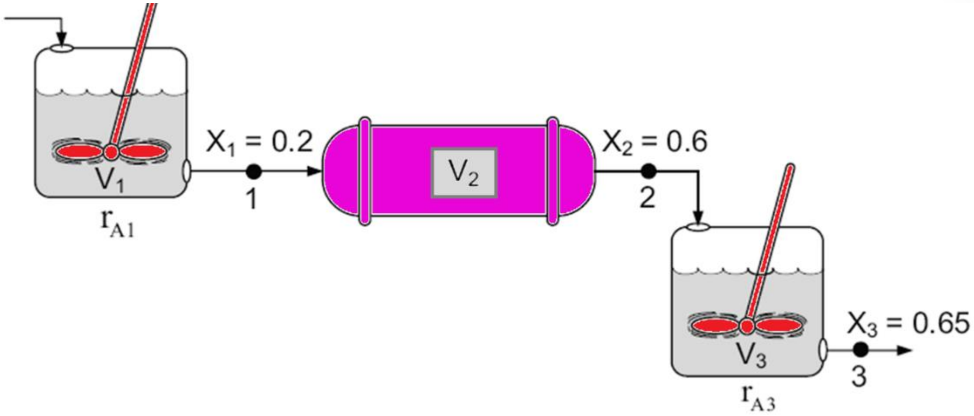
$$X_i = \frac{\text{total moles of A reacted up to point i}}{\text{moles of A fed to first reactor}}$$

Only valid if there are NO side streams.

- Molar Flow rate of species A at point i:

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

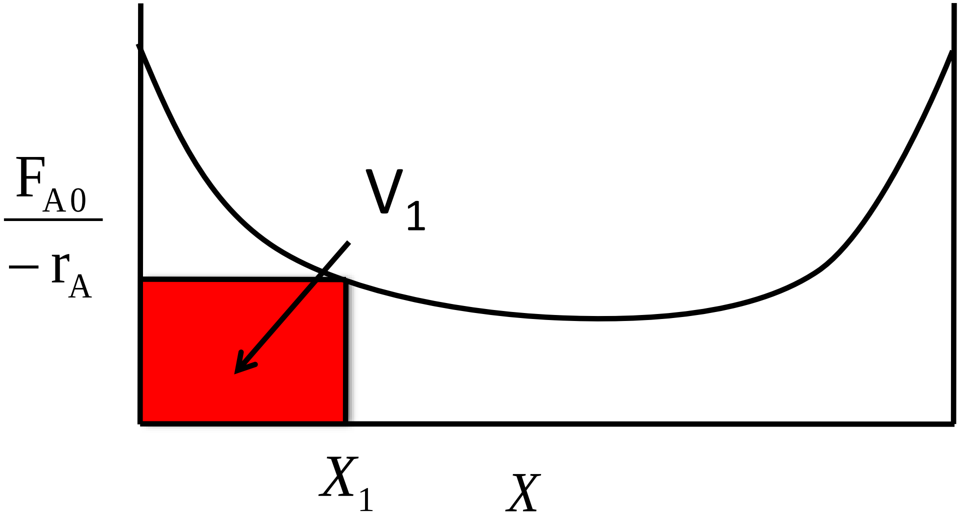
Reactors in Series



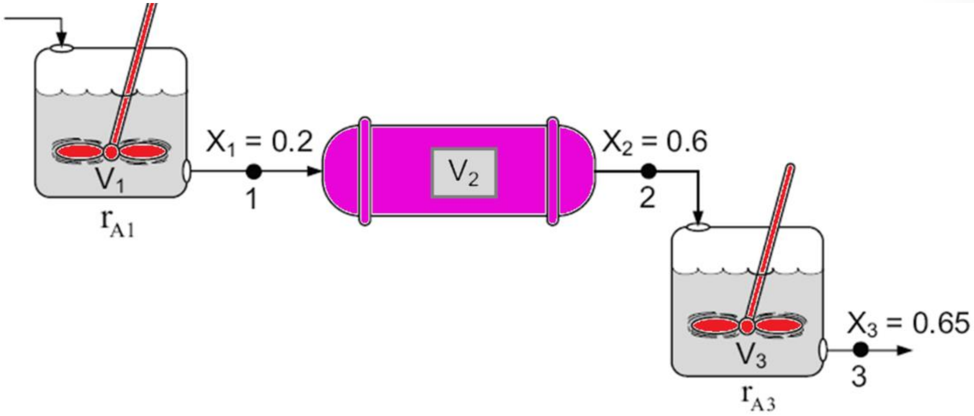
Reactor 1:

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

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

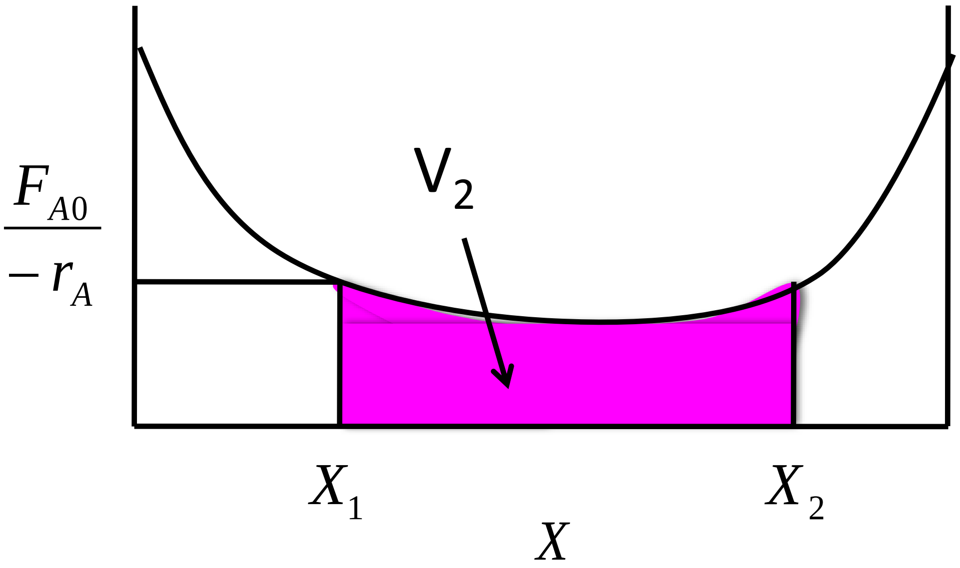


Reactors in Series

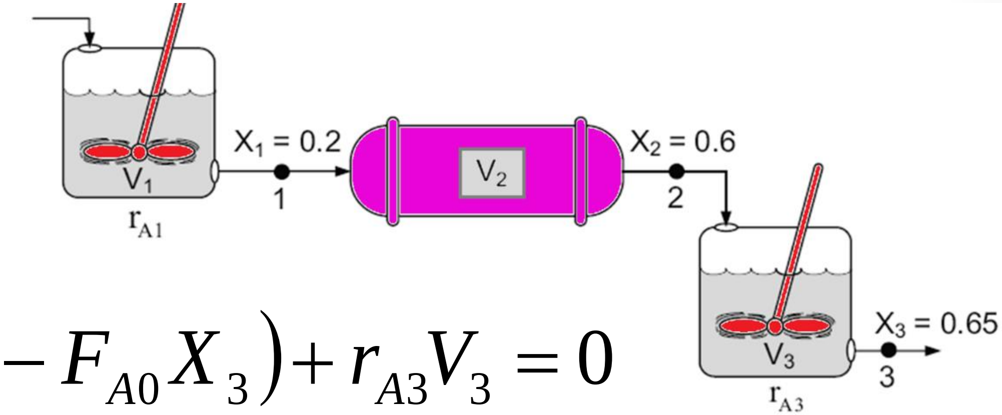


Reactor 2:

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



Reactors in Series

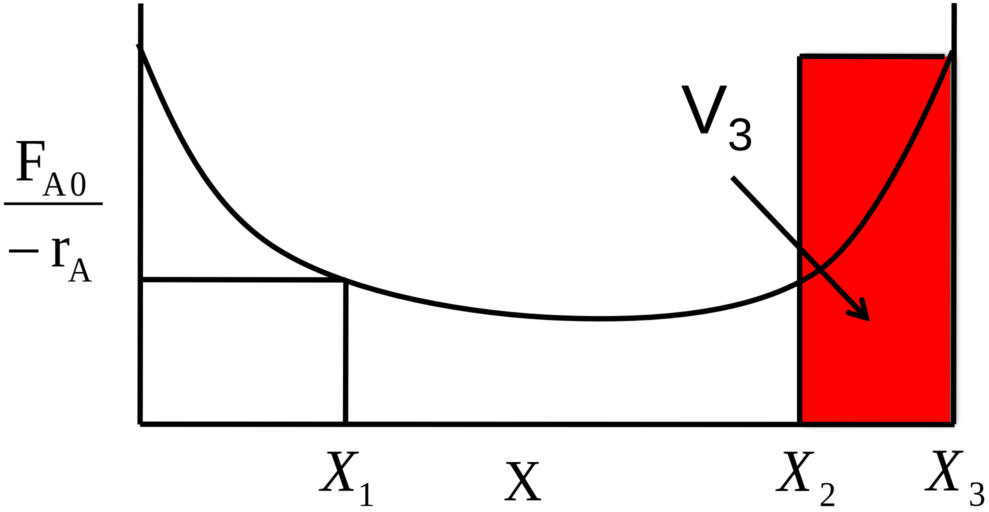


Reactor 3:

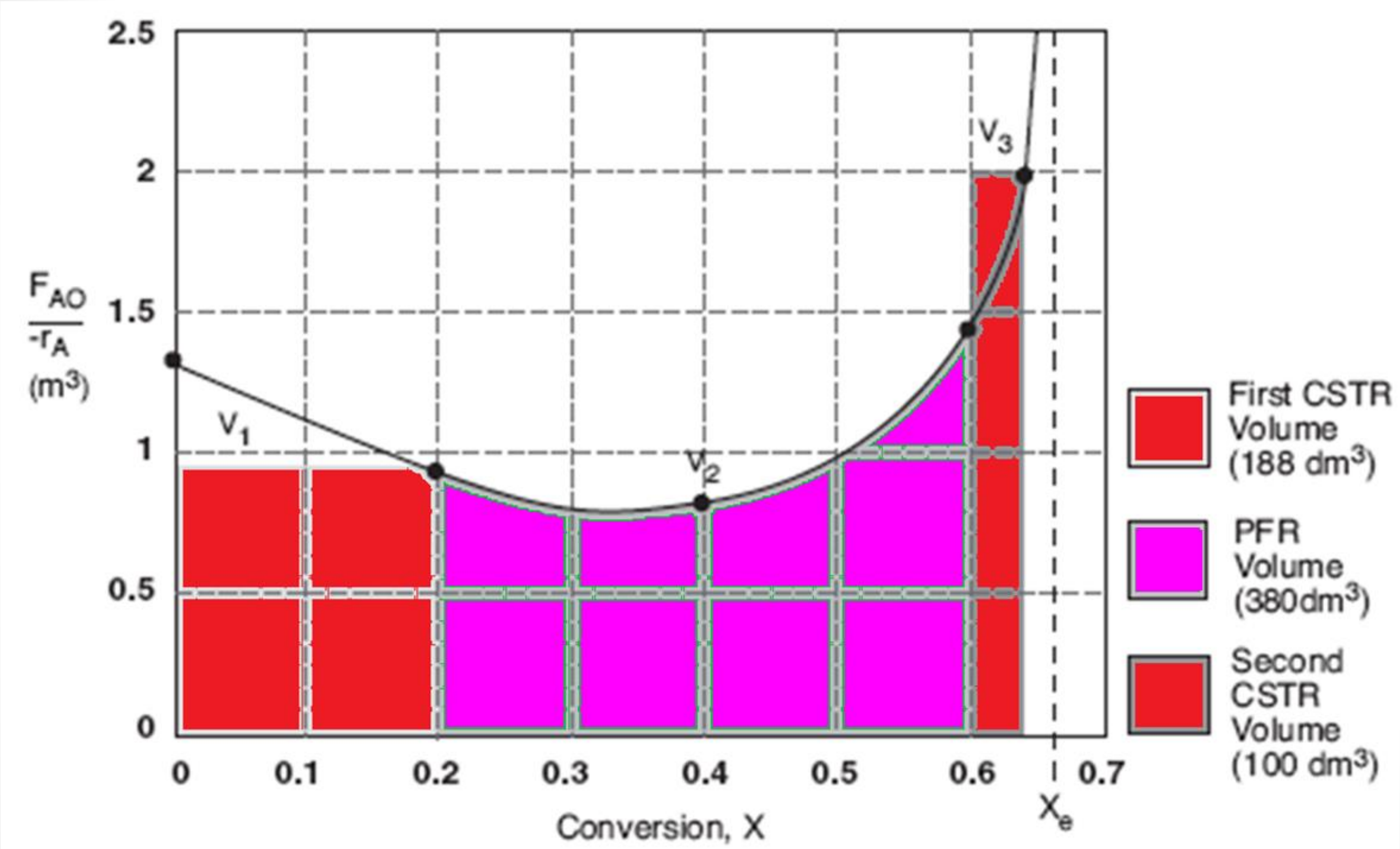
$$F_{A2} - F_{A3} + r_{A3}V_3 = 0$$

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

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



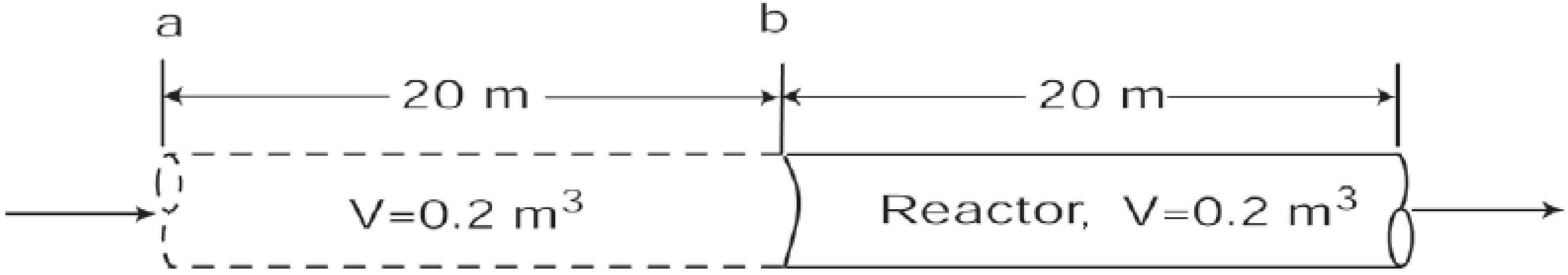
Reactors in Series



Space Time, τ

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

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



Space Velocity

- Defined as:

$$SV \equiv \frac{v_0}{V} \qquad SV = \frac{1}{\tau}$$

- Two space velocities commonly used in industry are:
  - **liquid-hourly space velocity, LHSV**

$$LHSV = \frac{v_{0|liquid}}{V}$$

  - **gas-hourly space velocity, GHSV**

$$GHSV = \frac{v_{0|STP}}{V}$$