



CHE 402

Kinetics & Reactor Design

Dr. Eid Al-Mutairi

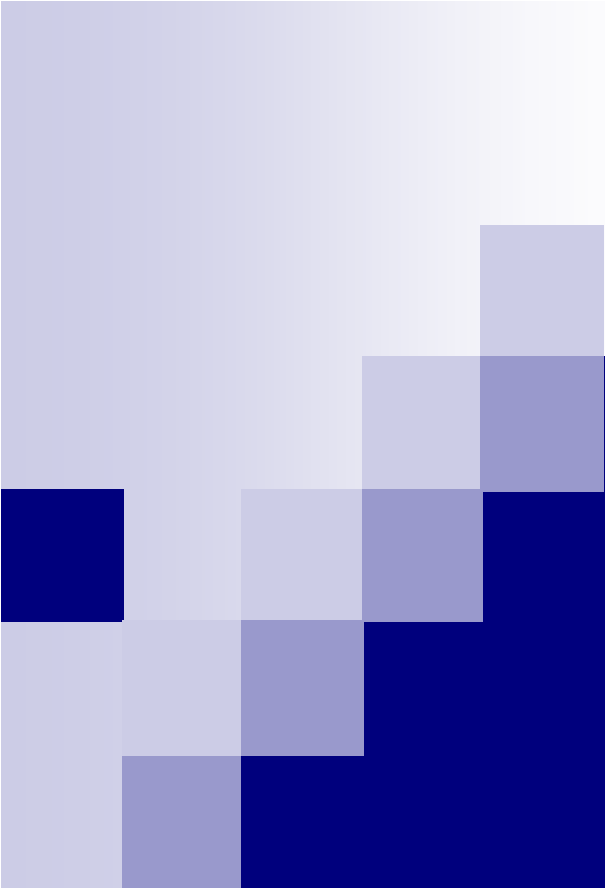


Announcements

■ **Quiz**

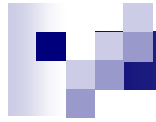
Oct. 29th

Material: Chapters 1&2



Chapter 2: Conversion and Reactor Sizing

Dr. Eid Al-Mutairi



Reactor Sizing

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The PFR volume necessary to achieve a conversion of X can also be calculated with a graphical technique. However, in the PFR's case, the integral form of the design equation

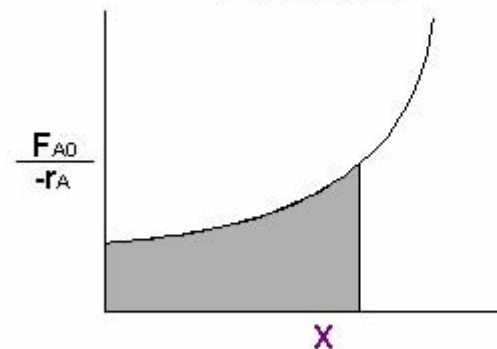
$$V = F_{A0} \int_0^X \frac{dX}{-r_A}$$

For a PFR, like a CSTR, $-r_A$ must be known as a function of conversion (X). (Remember, for a PFR, conversion varies down the length of a reactor)

$$V = \int_0^X \frac{F_{A0}}{-r_A} dX = \text{Area under the curve}$$



PFR System



Previous

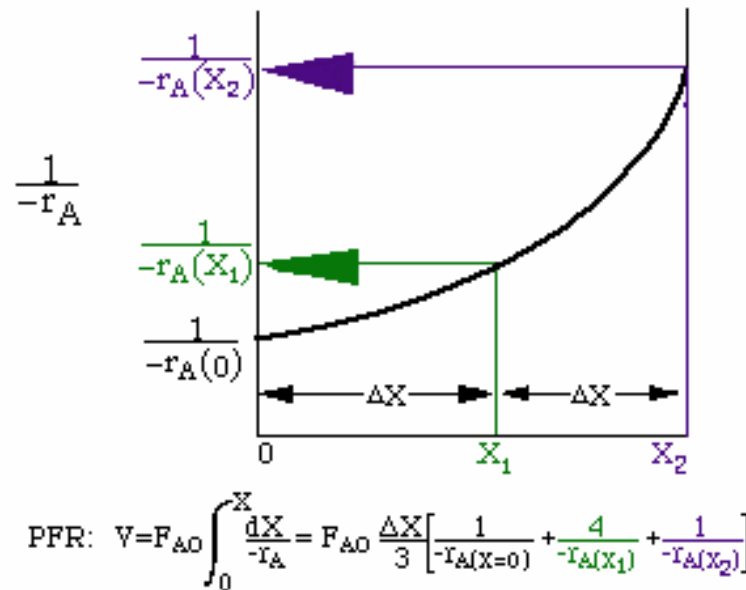
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Numerical Evaluation of Integrals

- The integral to calculate the PFR volume can be evaluated using Simpson's One-Third Rule (see Appendix A.4 on p. 1013):



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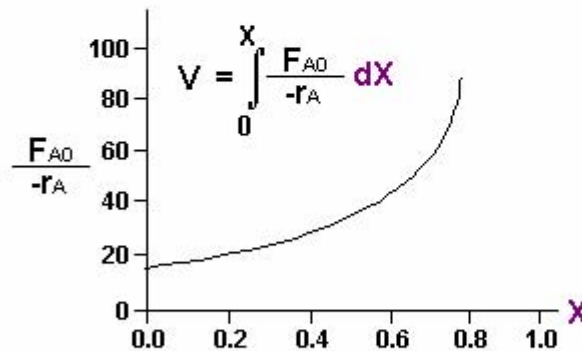
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To calculate the value of the integral, Simpson's one-third rule or Simpson's three-eighths rule could be used.

Simpson's Rules are algebraic expressions involving data for the graph. The one-third rule, which should only be used for linear portions of the graph, requires three data points. The three-eighths rule is more accurate and requires four data points.

Let's take a look at the one-third rule. Remember, this is only good for small portions of the graph.

x	f(x)
0.0	17
0.15	19
0.2	20
0.3	24
0.4	28
0.6	45



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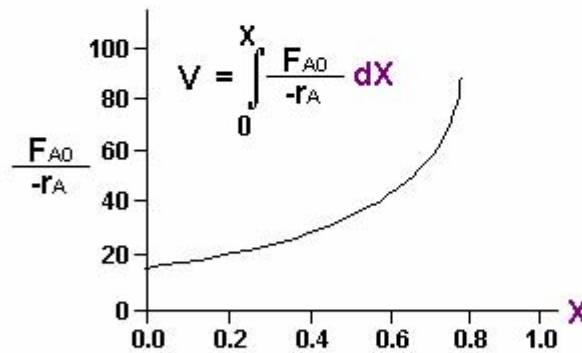
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Simpson's one-third rule:

$$\int_{X_0}^{X_2} f(X) dX = \frac{h}{3} [f(X_0) + 4 \cdot f(X_1) + f(X_2)]$$

$$h = \frac{X_2 - X_0}{2} \text{ and } X_1 = X_0 + h$$

X	f(x)
0.0	17
0.15	19
0.2	20
0.3	24
0.4	28
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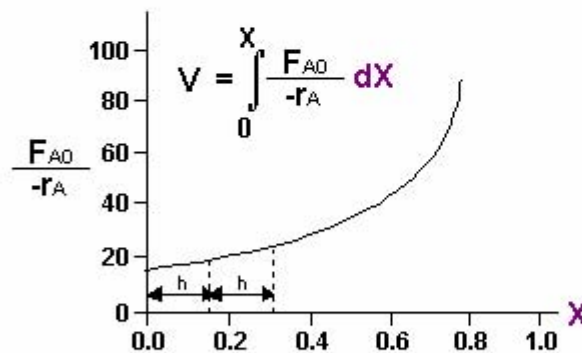
$$h = \frac{X_2 - X_0}{2} \text{ and } X_1 = X_0 + h$$

The volume required for a conversion of 0.3 would be calculated as follows:

$$X_0 = 0.0 \quad \text{So, } h = 0.15 \text{ and } X_1 = 0.15$$

$$X_2 = 0.3$$

X	f(x)
0.0	17
0.15	19
0.2	20
0.3	24
0.4	28
0.6	45



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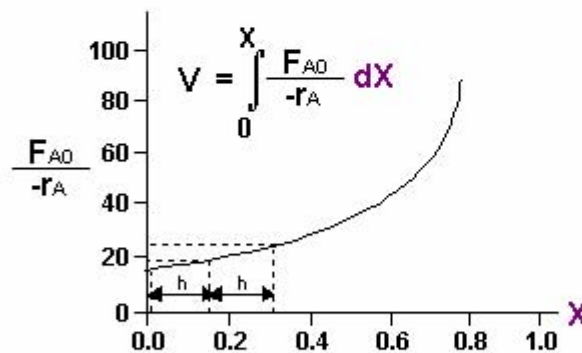
$$X_0 = 0.0 \quad \text{So, } h = 0.15 \text{ and } X_1 = 0.15$$

$$X_2 = 0.3 \quad f(X_0) = 17 \quad f(X_1) = 19 \quad f(X_2) = 24$$

$$V = \int_0^{0.3} f(X) dX = \frac{0.15}{3} [17 + 4(19) + 24]$$

$$V = 5.85 \text{ Liters}$$

X	f(x)
0.0	17
0.15	19
0.2	20
0.3	24
0.4	28
0.6	45



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The volume required for a conversion of 0.3 would be calculated as follows:

$$X_0 = 0.0 \quad \text{So, } h = 0.15 \text{ and } X_1 = 0.15$$

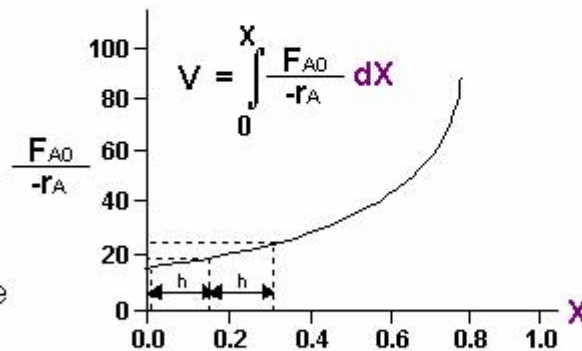
$$X_2 = 0.3 \quad f(X_0) = 17 \quad f(X_1) = 19 \quad f(X_2) = 24$$

$$V = \int_0^{0.3} f(X) dX = \frac{0.15}{3} [17 + 4(19) + 24]$$

$$V = 5.85 \text{ Liters}$$

Now, let's look at the three-eighths rule.

X	f(x)
0.0	17
0.15	19
0.2	20
0.3	24
0.4	28
0.6	45



Previous

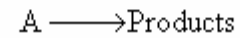
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Example

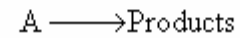
Consider the liquid phase reaction



which is to take place in a PFR. The following data was obtained in a batch reactor.

Example

Consider the liquid phase reaction



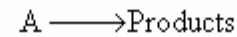
which is to take place in a PFR. The following data was obtained in a batch reactor.

$$V = F_{A0} \int_0^X \left(\frac{1}{-r_A} \right) dX$$

X	0	0.4	0.8
$-r_A$ (mol / dm ³ · s)	0.01	0.008	0.002

Example

Consider the liquid phase reaction



which is to take place in a PFR. The following data was obtained in a batch reactor.

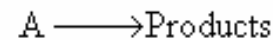
$$V = F_{A0} \int_0^X \left(\frac{1}{-r_A} \right) dX$$

X	0	0.4	0.8
$-r_A \text{ (mol / dm}^3 \cdot \text{s)}$	0.01	0.008	0.002
↓			
$\frac{1}{-r_A} \left(\frac{\text{dm}^3 \cdot \text{s}}{\text{mol}} \right)$	100	125	500

Construct a
Levenspiel Plot
 $\frac{1}{-r_A}$ vs. X

Example

Consider the liquid phase reaction



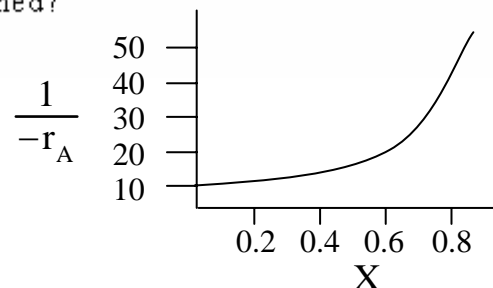
which is to take place in a PFR. The following data was obtained in a batch reactor.

$$V = F_{A0} \int_0^X \left(\frac{1}{-r_A} \right) dX$$

X	0	0.4	0.8
$-r_A$ (mol / dm ³ · s)	0.01	0.008	0.002
↓			
$\frac{1}{-r_A}$ (dm ³ · s / mol)	100	125	500

Construct a
Levenspiel Plot
 $\frac{1}{-r_A}$ vs. X

If the molar feed rate of A to the PFR is 2 mol/s, what volume is necessary to achieve 80% conversion under identical conditions as those under which the batch data obtained?



Solution

$$F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = F_{A0} \frac{h}{3} [f(X_0) + 4 * f(X_1) + f(X_2)]$$

Solution

$$F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = F_{A0} \frac{h}{3} [f(X_0) + 4 * f(X_1) + f(X_2)]$$

h=0.4 X0=0 X1=0.4 X2=0.8

Solution

$$F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = F_{A0} \frac{h}{3} [f(X_0) + 4 * f(X_1) + f(X_2)]$$

$$h=0.4 \quad X_0=0 \quad X_1=0.4 \quad X_2=0.8$$

$$V = F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = 2 \frac{0.4}{3} [f(0) + 4 * f(0.4) + f(0.8)]$$

Solution

$$F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = F_{A0} \frac{h}{3} [f(X_0) + 4 * f(X_1) + f(X_2)]$$

$$h=0.4 \quad X_0=0 \quad X_1=0.4 \quad X_2=0.8$$

$$V = F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = 2 \frac{0.4}{3} [f(0) + 4 * f(0.4) + f(0.8)]$$

$$V = F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = 2 \frac{0.4}{3} [100 + 4 * 125 + 500]$$

Solution

$$F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = F_{A0} \frac{h}{3} [f(X_0) + 4 * f(X_1) + f(X_2)]$$

$$h=0.4 \quad X_0=0 \quad X_1=0.4 \quad X_2=0.8$$

$$V = F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = 2 \frac{0.4}{3} [f(0) + 4 * f(0.4) + f(0.8)]$$

$$V = F_{A0} \int_0^{0.8} \frac{dX}{-r_A} = 2 \frac{0.4}{3} [100 + 4 * 125 + 500]$$

$$V=293.3 \text{ L}$$

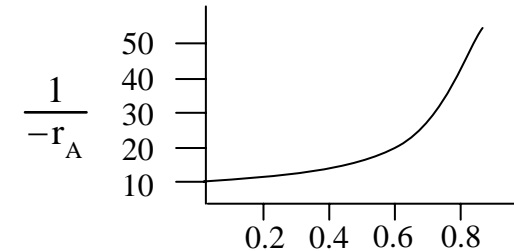


Example 2-2 [PFR]

Reactor Sizing- Summary

- 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.

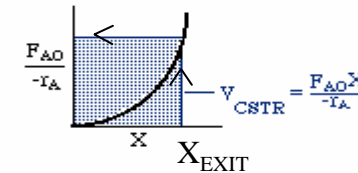


- Here we plot either $\frac{F_{A0}}{-r_A}$ or $\frac{1}{-r_A}$ as a function of X.

- For $\frac{F_{A0}}{-r_A}$ vs. X, the volume of a CSTR is:

$$V = \frac{F_{A0}(X-0)}{-r_A|_{EXIT}}$$

CSTR

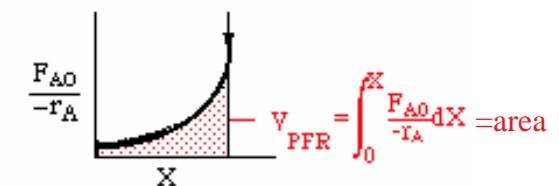


Equivalent to area of rectangle on a Levenspiel Plot

- For $\frac{F_{A0}}{-r_A}$ vs. X, the volume of a PFR is:

$$V_{PFR} = \int_0^X \frac{F_{A0}}{-r_A} dX = \text{area under the curve}$$

PFR





Reactor Staging

Reactors In Series

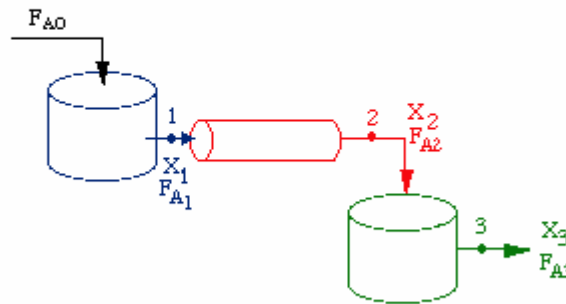
$$X_i = \frac{\text{moles of A reacted up to point i}}{\text{moles of A fed to first reactor}}$$

Only valid if there are no side streams

Reactors In Series

$$X_i = \frac{\text{moles of A reacted up to point i}}{\text{moles of A fed to first reactor}} \quad \text{Only valid if there are no side streams}$$

Consider a PFR between two CSTRs

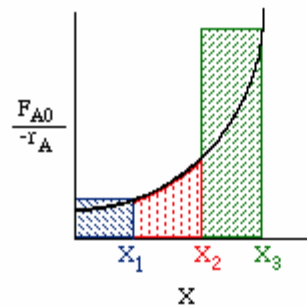
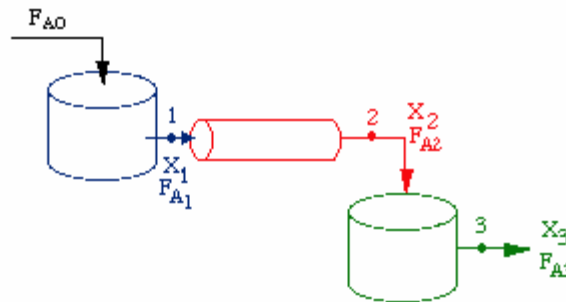


Reactors In Series

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

Only valid if there are no side streams

Consider a PFR between two CSTRs



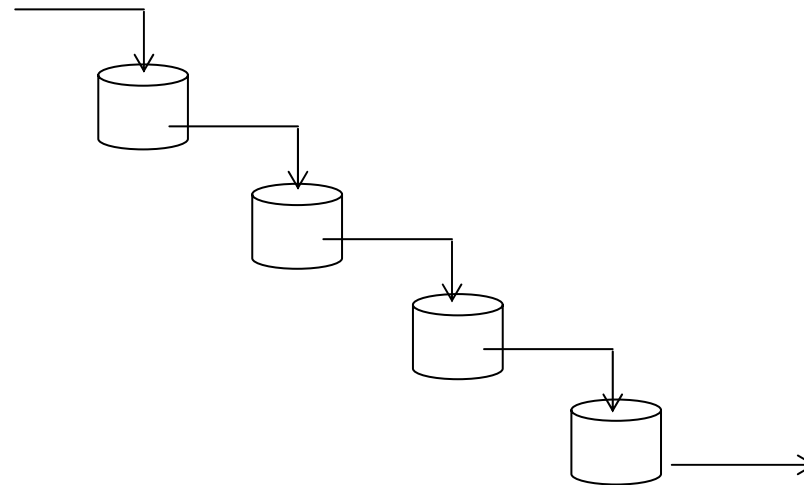
$$V_1 = \frac{F_{A0} X_1}{-r_{A1}}$$

$$V_2 = \int_{X_1}^{X_2} \frac{F_{A0}}{-r_{A2}} dX$$

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

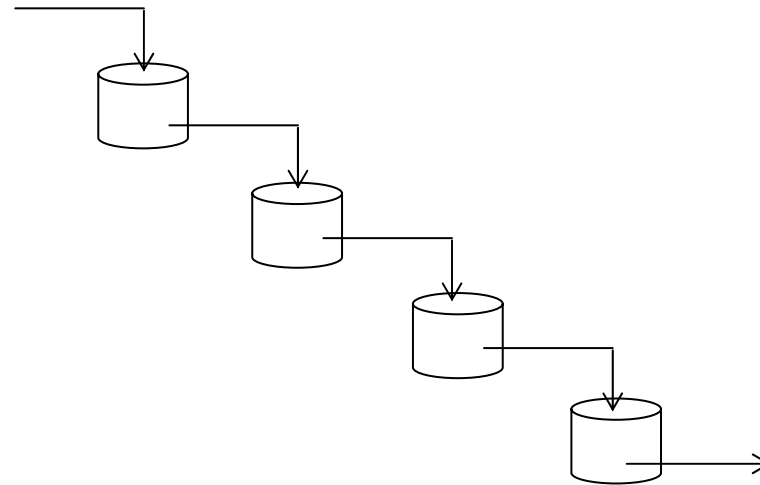
Reactors in Series

- Also consider a number of CSTRs in series:



Reactors in Series

- Finally consider a number of CSTRs in series:



- We see that we approach the PFR reactor volume for a large number of CSTRs in series:

