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

Staging

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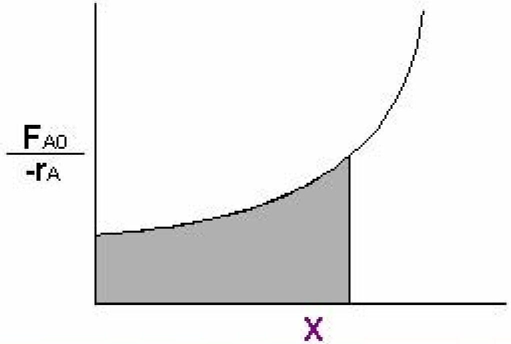
The PFR volume necessary to achieve a conversion of X can also be calculated with a graphical technique. However, in the PFR's case, the integral form of the design equation

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

For a PFR, like a CSTR, -rA 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



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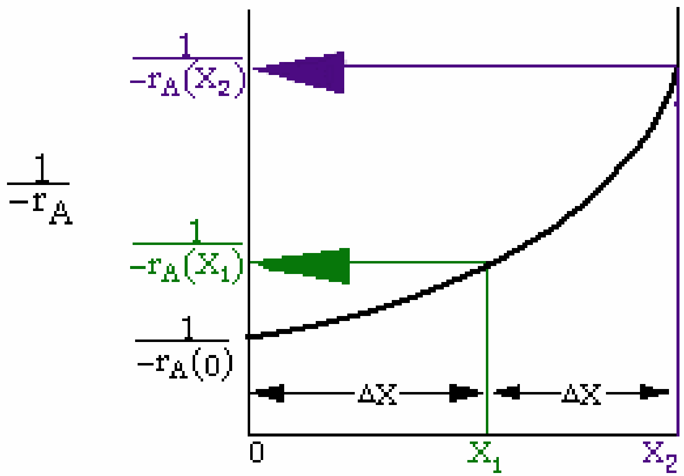
Numerical Evaluation of Integrals

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



$$\text{PFR:}\quad V = F_{A0}\int_0^X \frac{dX}{-r_A} = F_{A0}\frac{\Delta X}{3}\left[\frac{1}{-r_{A(X=0)}} + \frac{4}{-r_{A(X_1)}} + \frac{1}{-r_{A(X_2)}}\right]$$

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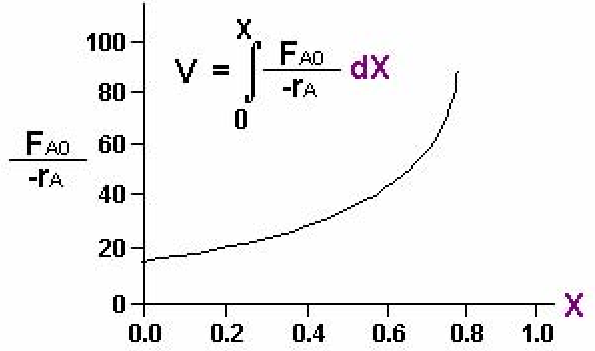
To calculate the value of the integral, Simpson's one-third rule or Simpson's three-eights rule could be used.

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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Simpson's one-third rule:

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

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

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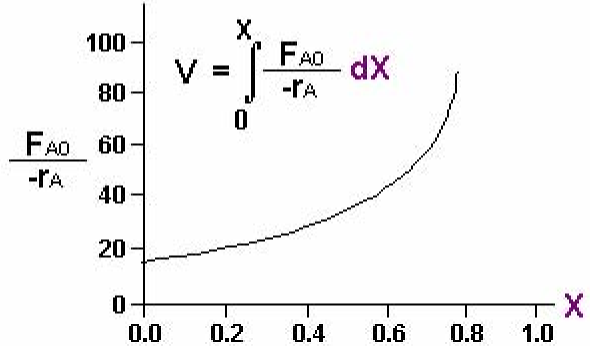

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The volume required for a conversion of 0.3 would be calculated as follows:

$X_0 = 0.0$
$X_2 = 0.3$ So, $h = 0.15$ and $X_1 = 0.15$

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0.2	20
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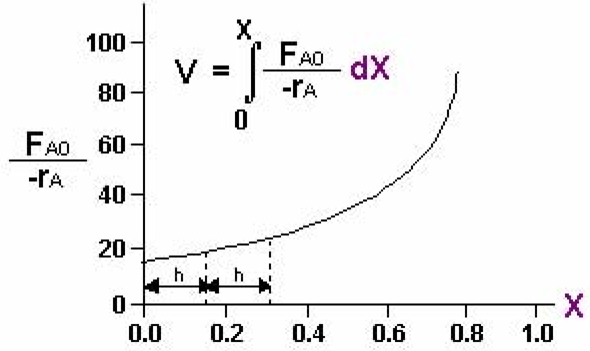

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$$V = \int_0^{0.3} f(X)\,dX = \frac{0.15}{3}\left[17 + 4(19) + 24 \right]$$

$V = 5.85$ Liters

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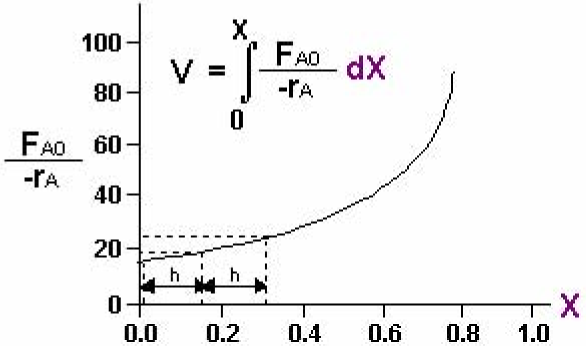

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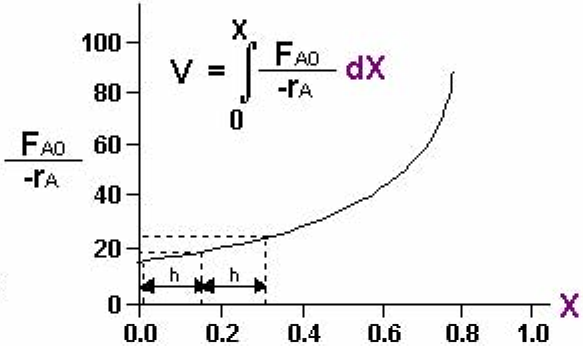

Now, let's look at the three-eighths rule.

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Example

Consider the liquid phase reaction

$$A \longrightarrow \text{Products}$$

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

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

X	0	0.4	0.8
$-r_A\,(mol/dm^3 \cdot s)$	**0.01**	0.008	0.002

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$\frac{1}{-r_A} \left(\frac{dm^3 \cdot s}{mol} \right)$	100	125	500

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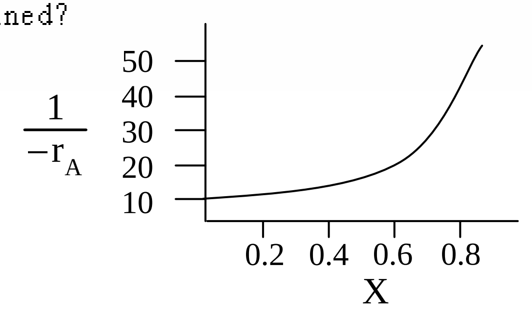
Construct a Levenspiel Plot $\frac{1}{-r_A}$ vs. X

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

$$F_{A0}\int_{0}^{0.8}\frac{dX}{-r_A}=F_{A0}\frac{h}{3}\left[f(X_0)+4*f(X_1)+f(X_2)\right]$$

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$$F_{A0}\int_{0}^{0.8}\frac{dX}{-r_A}=F_{A0}\frac{h}{3}\left[f(X_0)+4*f(X_1)+f(X_2)\right]$$

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

Solution

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

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

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

Solution

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

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

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

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

Solution

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

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

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

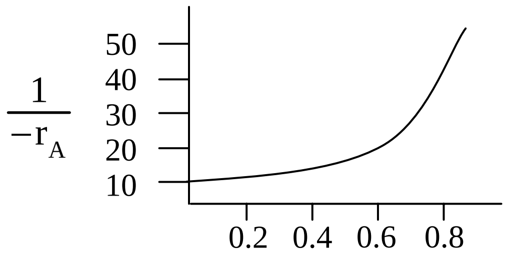
$$V=F_{A0}\int_0^{0.8}\frac{dX}{-r_A}=2\frac{0.4}{3}\left[100+4*125+500\right]$$

V=293.3 L

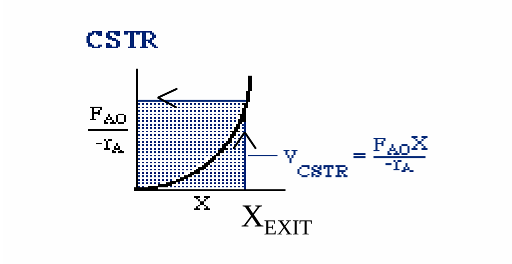
Example 2-2 [PFR]

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.



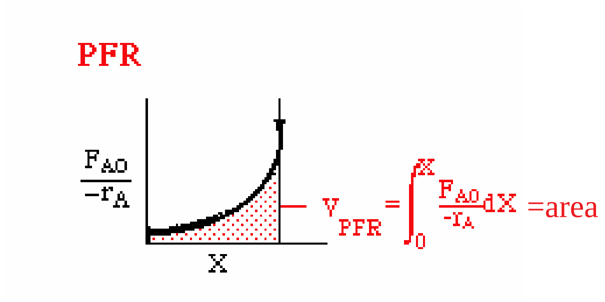
Equivalent to area of rectangle on a Levenspiel Plot

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

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

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

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



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

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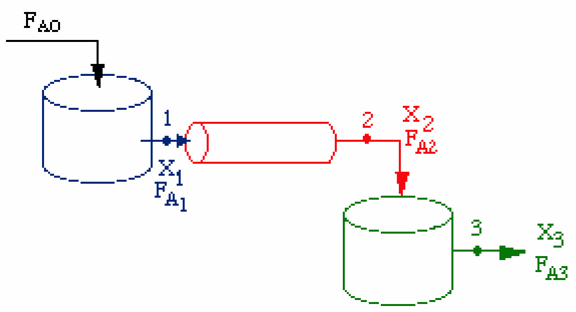
Consider a PFR between two CSTRs



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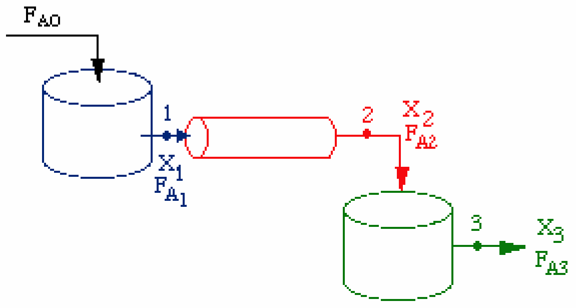
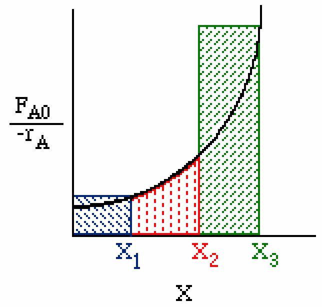




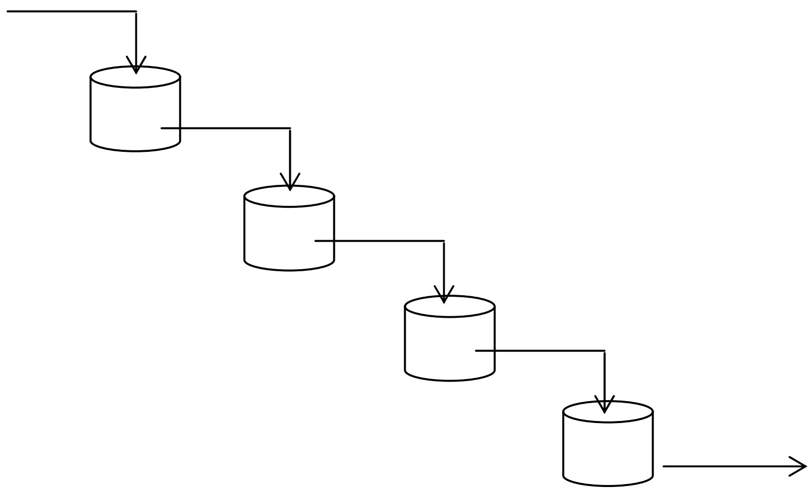
$$V_1 = \frac{F_{A0}X_1}{-r_{A_1}}$$

$$V_2 = \int_{X_1}^{X_2} \frac{F_{A0}}{-r_{A_2}} dX$$

$$V_3 = \frac{F_{A0}(X_3 - X_2)}{-r_{A_3}}$$

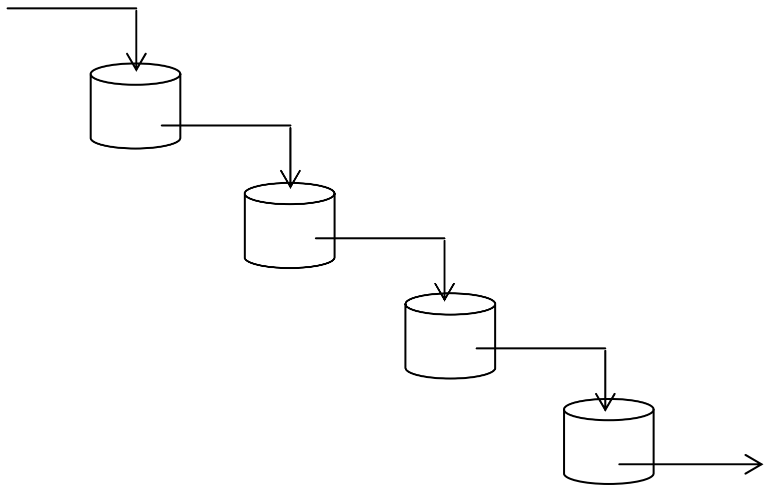
Reactors in Series

- 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: