CHEMICAL REACTOR DESIGN

CHENG 323

Dr Shaker Haji

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2 Conversion & Reactor Sizing

Prepared by: Dr Shaker Haji - CHENG 323

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Lecture 6

- Define Conversion, X
- Develop the Design Eqns. in Terms of X
- Size CSTR

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Reflections خواطر

The subject of chemical reaction engineering (CRE) was initiated and evolved primarily to accomplish the task of ***describing,*** for a given reactive system, ***how to***:

- choose the proper reactor,
- calculate its size, and
- determine its optimal operating conditions.

Mark E. Davis and Robert J. Davis, Fundamentals of Chemical Reaction Engineering.

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In this Chapter

In the first chapter, the general mole balance equation was derived and then applied to the four most common types of industrial reactors (ideal reactors).

In this Chapter:

Define Conversion, X
Develop the Design Equations in Terms of X
Size CSTRs and PFRs given $-r_A$ vs. X
Compare Conversions for Reactors in Series

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2.1 Definition of Conversion

- In defining conversion, we choose one of the reactants, the limiting reactant, as the basis of calculations.

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

Choose the limiting reactant, A, as basis of calculation:

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

Now, every quantity is on a "per mole of A" basis.

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2.1 Definition of Conversion

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

The conversion, X_A, is defined as:

$$X_A = \frac{\text{moles A reacted}}{\text{moles A fed}}, \qquad X \equiv X_A$$

- For irreversible rxns, the max. conversion is 1.
- For reversible rxns, the max. conversion is the equilibrium conversion, X_e.
- If A is the limiting reactant and B is provided in excess, can X_B reach 1 (100% conversion of B)?

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2.2 Batch Reactor Design Equations

In most batch reactors, the longer a reactant stays in the reactor, the more the reactant is converted to products until:

1. either equilibrium is reached
2. or the limiting reactant is exhausted.

Write X equation symbolically. $X_A = \frac{\text{moles A reacted}}{\text{moles A fed}}$

$$X = \frac{N_{A0} - N_A}{N_{A0}} \qquad \rightarrow \qquad N_A = N_{A0}(1 - X)$$

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2.2 Batch Reactor Design Equations

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

Starting from the general mole balance equation, derive the batch reactor design equation in terms of *X*.

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2.2 Batch Reactor Design Equations

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

Differential Form of Batch Mole Balance Eq.
Used for interpretation of rxn rate data

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

Differential Form of Batch Design Eq.
Usually used for finding *V*

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

Integral Form of Batch Design Equation
Usually used for finding *t*

The longer the reactants are left in the reactor, the greater will be the conversion.

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2.3 Design Equations for Flow Reactors

15 min

- For a batch reactor, *X* increases with time spent in the reactor.
- For continuous-flow systems, this time usually increases with increasing reactor volume.
- The bigger the reactor, the more time it will take the reactants to flow completely through the reactor and thus, the more time to react.
- Therefore, *X* = *f* (*V*)
- For continuous-flow sys., *X* can be defined mathematically as

$$X_A = \frac{\text{moles A reacted}}{\text{moles A fed}} = \frac{F_{A0} - F_A}{F_{A0}} \qquad \therefore F_A = F_{A0}(1 - X)$$

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2.3 Design Equations for Flow Reactors

Recall that: $F_{A0} = C_{A0} \cdot \upsilon_0$

- For liquid systems, C_{A0} is given is terms of molarity
- For gas systems, C_{A0} can be calculated from an applicable EOS
- For gas systems at high *T* & low *P*, C_{A0} can be calculated from:

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

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2.3.1 Design Equation for CSTR

Starting from the general mole balance equation, derive the CSTR design equation in terms of X.

$$F_{i0} - F_i + \int_0^V r_i \cdot dV = \frac{dN_i}{dt} \Rightarrow V = \frac{F_{A0} - F_A}{-r_A\big|_{exit}} \Rightarrow V = \frac{F_{A0}X}{-r_A\big|_{exit}}$$

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2.3.1 Design Equation for CSTR

Starting from the general mole balance equation, derive the CSTR design equation in terms of X.

$$F_{i0} - F_i + \int_0^V r_i \cdot dV = \frac{dN_i}{dt} \Rightarrow V = \frac{F_{A0} - F_A}{-r_A\big|_{exit}} \Rightarrow V = \frac{F_{A0}X}{-r_A\big|_{exit}}$$

- Because the CSTR is perfectly mixed, the exit composition is identical to that inside the reactor.
- Therefore, the rate of rxn is evaluated at the exit conditions.

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2.3.2 Plug Flow Reactor (PFR)

- As the reactants enter and flow axially down the reactor, they are consumed and the *X* increases along the length of the reactor.

Starting from the PFR design equation, derive the PFR design equation in terms of *X*.

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

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2.3.2 Plug Flow Reactor (PFR)

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

Differential Form of PFR Mole Balance Eq. in terms of molar flow rate

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

Differential Form of PFR Design Eq. in terms of X.

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

Integral Form of PFR Design Equation in terms of X.

What is needed in order to integrate the above eq.?

We need to know the $r_A = f(X)$ [Chap 3]

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2.3.3 Packed-Bed Reactor (PBR)

- Packed-bed reactors are tubular reactors filled with catalyst particles.
- The PBR design equation in terms of X will be:

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

Differential Form of PBR Design Eq. in terms of X.

- The differential form **must** be used when analyzing reactors that have ΔP along the length of the reactor [Chap 4].
- If $\Delta P = 0$, the integral form can be used:

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

Integral Form of PBR Design Equation

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2.4 Applications of the Design Equations for Continuous-Flow Reactors

Now, we are going to show how to size CSTRs & PFRs from knowledge of r_A at different X_A ($-r_A$ vs. X).

Consider the isothermal gas-phase isomerization: **A→B**

- You are asked to go to the lab to study how the rate of rxn changes as the rxn proceeds (i.e. find $-r_A$ vs. X_A).

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2.4 Applications of the Design Equations for Continuous-Flow Reactors

- For **A→ B**, find $-r_A$ vs. X_A
- The experiment shall be carried out – in a batch reactor – under an isothermal (T = 500 K), isobaric (830 kPa), & isochoric condition with y_{A0}=1.
- What shall be measured and calculated?

t	C_A	X_A	$-r_A$

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Recall the DE of CSTR & PFR:

$$V = \frac{F_{A0}X}{-r_A\big|_{exit}} \qquad V = F_{A0}\int_0^X \frac{dX}{-r_A}$$

What is V proportional to,
$-r_A$ or $(1/-r_A)$?

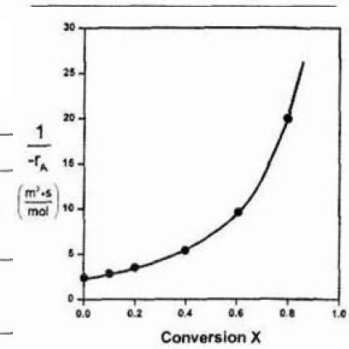
Levenspiel Plot

TABLE 2-1 RAW DATA

X	$-r_A$ (mol/m³ · s)
0	0.45
0.1	0.37
0.2	0.30
0.4	0.195
0.6	0.113
0.7	0.079
0.8	0.05

TABLE 2-2 PROCESSED DATA –1

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{\text{m}^3\cdot\text{s}}{\text{mol}}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20



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$$V = \frac{F_{A0}X}{-r_A\big|_{exit}}$$

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

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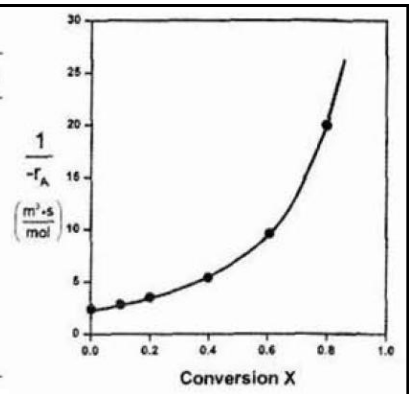

- This Fig. can be used to size flow reactors for different F_{A0}.
- Before sizing flow reactors let's get some insights into this Fig.

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$$V = \frac{F_{A0}X}{-r_A\big|_{exit}}$$

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

TABLE 2-1 RAW DATA

X	$-r_A$ (mol/m³ · s)
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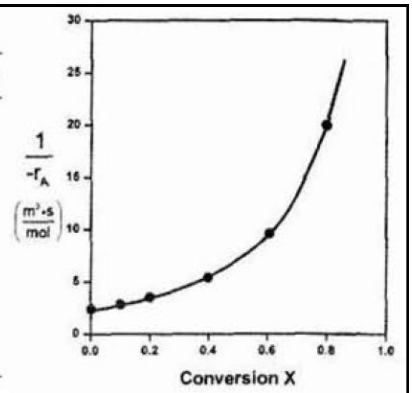

- For isothermal rxn, when the rate of rxn is greatest?
- What happens to the rate of rxn as the reaction progresses?
- For irresversible rxns of greater than zero order, what is the V required to achieve complete conversion?

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

- For reversible rxns, what is max X ? What is $-r_A$ & V when $X=X_{eq}$?

$A \rightleftarrows B$ As $X \rightarrow X_e, -r_A \rightarrow 0$, thus, $\frac{1}{-r_A} \rightarrow \infty$ and therefore $V \rightarrow \infty$

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

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

In the following examples , we will use F_{A0} = 0.4 mol/s.

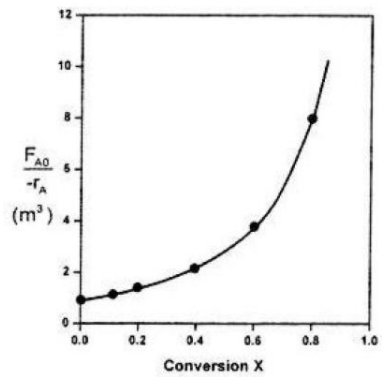

Figure 2-2 Levenspiel plot of processed data –2.

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{mol}{m^3 \cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{m^3 \cdot s}{mol}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](m^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

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Example 2-2 Sizing a CSTR

40 min

The previously discussed isothermal gas-phase isomerization rxn, A → B, is to be carried out in a CSTR. Species A enters the reactor at F_{A0} = 0.4 mol/s, y_{A0} = 1, C_{A0} = 0.2 mol/L, and υ_0 = 2 L/s.

1. Using the obtained kinetic data, calculate the volume necessary to achieve 80% conversion in a CSTR.

TABLE 2-3 PROCESSED DATA –2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{mol}{m^3 \cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{m^3 \cdot s}{mol}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](m^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

$$V = \left(\frac{F_{A0}}{-r_A\big|_{exit}}\right)\cdot X$$

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Example 2-2 Sizing a CSTR

The previously discussed rxn is to be carried out in a CSTR. Species A enters the reactor at $F_{A0} = 0.4$ mol/s.

2. Shade the area that would give the CSTR volume necessary to achieve 80% conversion.

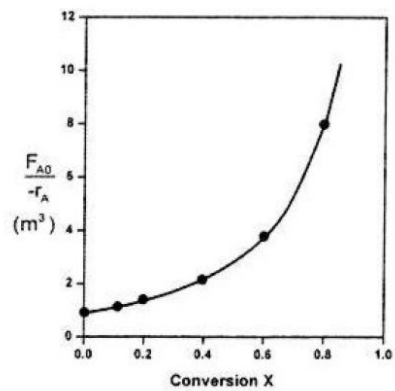

Figure 2-2 Levenspiel plot of processed data –2.

$$V = \left(\frac{F_{A0}}{-r_A\big|_{exit}} \right) \cdot X$$

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Example 2-2 Sizing a CSTR

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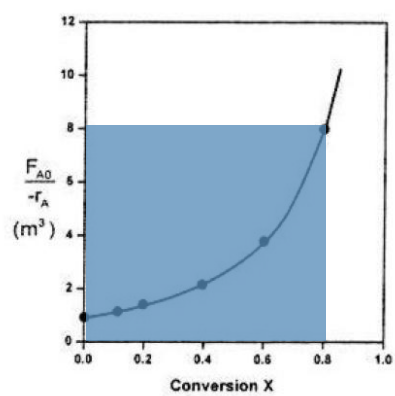

Figure 2-2 Levenspiel plot of processed data –2.

$$V = \left(\frac{F_{A0}}{-r_A\big|_{exit}} \right) \cdot X$$

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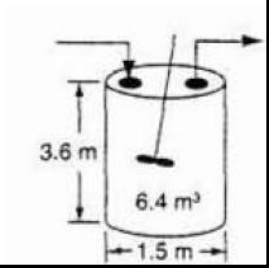
Example 2-2 Sizing a CSTR

- The CSTR volume necessary to achieve $X = 80\%$ is 6.4 m^3.
- This volume corresponds to a reactor about 1.5 m in diameter and 3.6 m high.
- It's a large CSTR, but this is a gas-phase reaction, and CSTRs are normally not used for gas-phase reactions.
- CSTRs are used primarily for liquid-phase reactions



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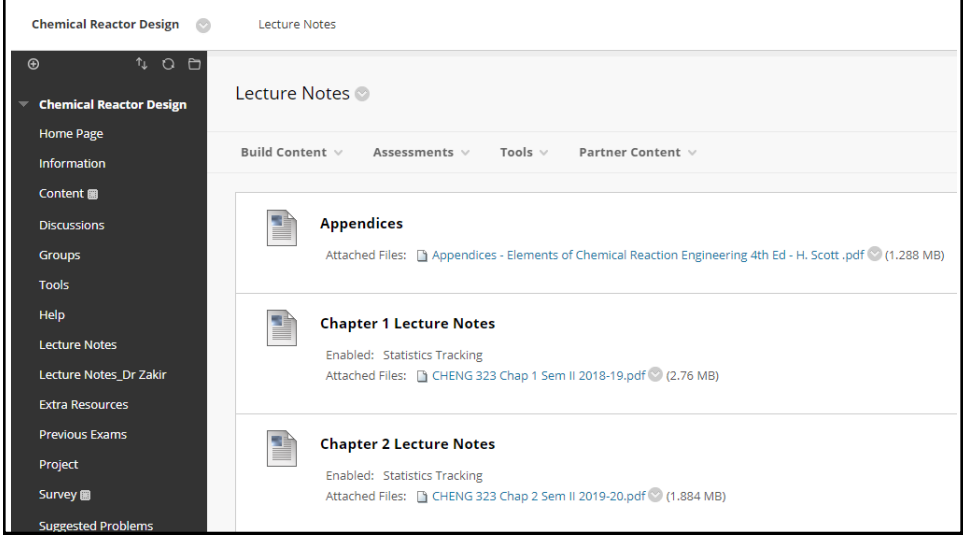
Please, bring a copy of the Appendices to the following lectures



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Lecture 7

- Sizing a PFR
- Comparing CSTR and PFR Sizes

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Example 2-3 Sizing a PFR

Isothermal gas-phase isomerization rxn: A → B.

The previously discussed rxn is to be carried out in a PFR. Species A enters the reactor at $F_{A0} = 0.4$ mol/s.

1. Shade the area in the $F_{A0}/-r_A$ vs. X figure that would give the PFR volume necessary to achieve 80% conversion.

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

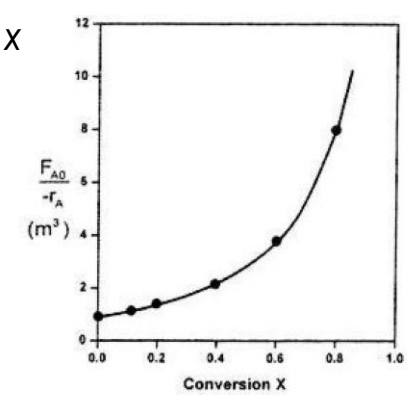

Figure 2-2 Levenspiel plot of processed data –2.

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Example 2-3 Sizing a PFR

The previously discussed rxn is to be carried out in a PFR. Species A enters the reactor at $F_{A0} = 0.4$ mol/s.

1. Shade the area in the $F_{A0}/-r_A$ vs. X figure that would give the PFR volume necessary to achieve 80% conversion.

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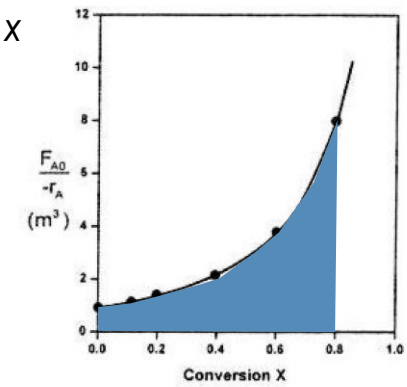

Figure 2-2 Levenspiel plot of processed data –2.

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Example 2-3 Sizing a PFR

The previously discussed rxn is to be carried out in a PFR. Species A enters the reactor at $F_{A0} = 0.4$ mol/s.

2. Use curve fitting, then analytical integration to determine the PFR volume necessary to achieve 80% conversion.

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

TABLE 2-3 PROCESSED DATA –2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A \left(\frac{\text{mol}}{\text{m}^3 \cdot \text{s}}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{\text{m}^3 \cdot \text{s}}{\text{mol}}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

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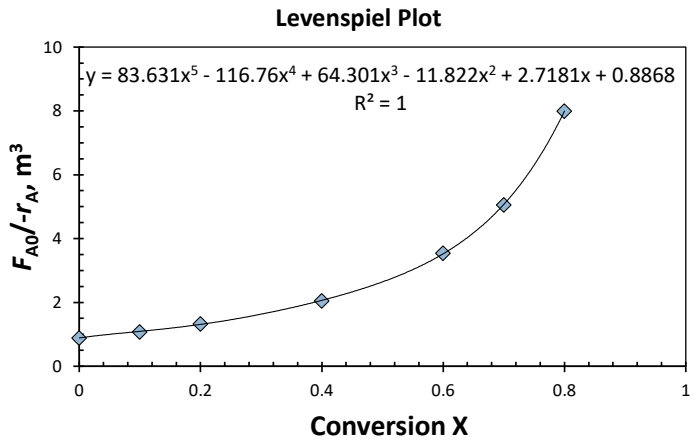

$$V = \int_0^X (83.631x^5 - 116.76x^4 + 64.301x^3 - 11.822x^2 + 2.7181x + 0.8868)\ dx$$

By curvefitting/analytical integration, V_{PFR} = 2.148 m^3.

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

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

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Example 2-3 Sizing a PFR

The previously discussed rxn is to be carried out in a PFR. Species A enters the reactor at F_{A0} = 0.4 mol/s.

3. Use a numerical integration method to determine the PFR volume necessary to achieve 80% conversion. (see Appendix A.4)

TABLE 2-3 PROCESSED DATA –2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{mol}{m^3 \cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{m^3 \cdot s}{mol}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](m^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

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

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A.4 Numerical Evaluation of Integrals

1. *Trapezoidal rule* (two-point) (Figure A-2). This method is one of the simplest and most approximate, as it uses the integrand evaluated at the limits of integration to evaluate the integral

$$\int_{X_0}^{X_1} f(X)\,dX = \frac{h}{2}[f(X_0)+f(X_1)] \qquad \text{(A-20)}$$

when $h = X_1 - X_0$.

2. *Simpson's one-third rule* (three-point) (Figure A-3). A more accurate evaluation of the integral can be found with the application of Simpson's rule:

$$\int_{X_0}^{X_2} f(X)\,dX = \frac{h}{3}[f(X_0)+4f(X_1)+f(X_2)] \qquad \text{(A-21)}$$

where

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

4. *Five-point quadrature formula.*

$$\int_{X_0}^{X_4} f(X)\,dX = \frac{h}{3}(f_0+4f_1+2f_2+4f_3+f_4) \qquad \text{(A-23)}$$

where

$$h = \frac{X_4 - X_0}{4}$$

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1. *Trapezoidal rule* (two-point) (Figure A-2). This method is one of the simplest and most approximate, as it uses the integrand evaluated at the limits of integration to evaluate the integral

$$\int_{X_0}^{X_1} f(X)\,dX = \frac{h}{2}[f(X_0)+f(X_1)] \qquad \text{(A-20)}$$

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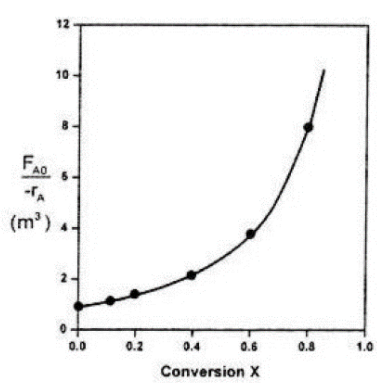
$$V = \int_0^X \left(\frac{F_{A0}}{-r_A}\right) dX$$



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$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

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4. *Five-point quadrature formula.*

$$\int_{X_0}^{X_4} f(X)\,dX = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4)$$

where $$h = \frac{X_4 - X_0}{4}$$

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$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

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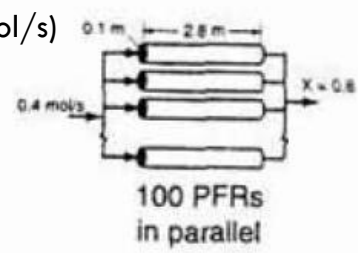
Example 2-3 Sizing a PFR

- The PFR reactor volume necessary to achieve 80% conversion is 2.165 m^3 (using five-point quadrature formula)
- This volume could result from a 0.1 m-diameter tubular reactor with a length of 276 m!
- or – a more realistic arrangement – from a bank of 100 PFRs that are each 0.1 m in diameter with a length of 2.76 m. (where each PFR processes $F_{A0}/100$ mol/s)



Exercise: find V_i (the volume of each reactor) and $V_{total,\ bank}$ then compare it to $V_{single,\ PFR}$

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Example 2-3 Sizing a PFR

30 min

The previously discussed rxn is to be carried out in a PFR. Species A enters the reactor at $F_{A0} = 0.4$ mol/s.

4. Make qualitative sketches of the X & $-r_A$ down the volume of the reactor.

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

TABLE 2-3 PROCESSED DATA –2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A \left(\frac{\text{mol}}{\text{m}^3 \cdot \text{s}}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{\text{m}^3 \cdot \text{s}}{\text{mol}}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

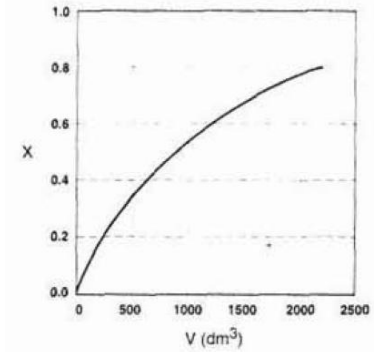
40

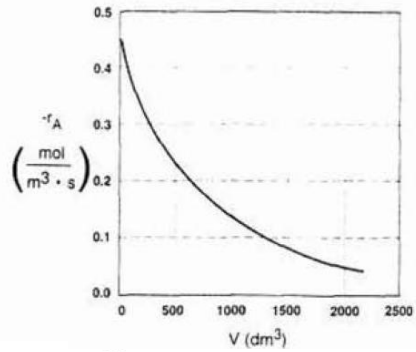
Example 2-3 Sizing a PFR

TABLE E2-3.1. CONVERSION AND REACTION RATE PROFILES

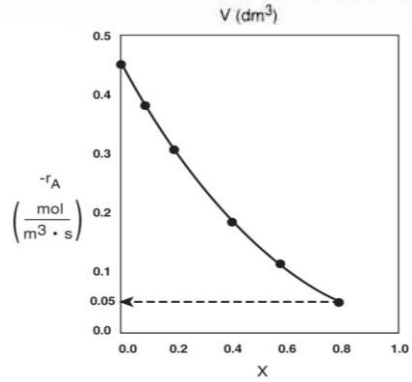
X	0	0.2	0.4	0.6	0.8
$-r_A \left(\frac{\text{mol}}{\text{m}^3 \cdot \text{s}}\right)$	0.45	0.30	0.195	0.113	0.05
V (dm^3)	0	218	551	1093	2165

41





- $-r_A$ decreases as we move down the reactor while X increases.
- These plots are typical for reactors operated isothermally.
- Also plot $-r_A$ vs. X.



42

Example 2-4 Comparing CSTR and PFR Sizes

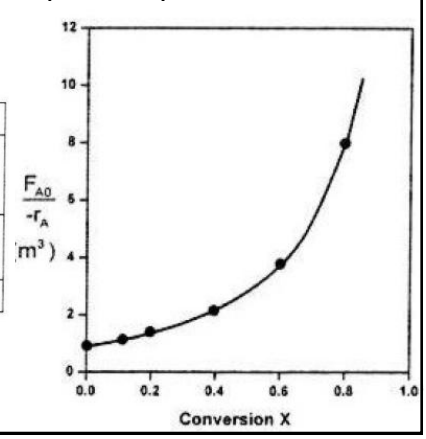
For the previous example, graphically compare the volumes of a CSTR & PFR required for the same job (X=80%).

TABLE 2-3 PROCESSED DATA –2

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{mol}{m^3 \cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A)\left(\frac{m^3 \cdot s}{mol}\right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$[F_{A0}/-r_A](m^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

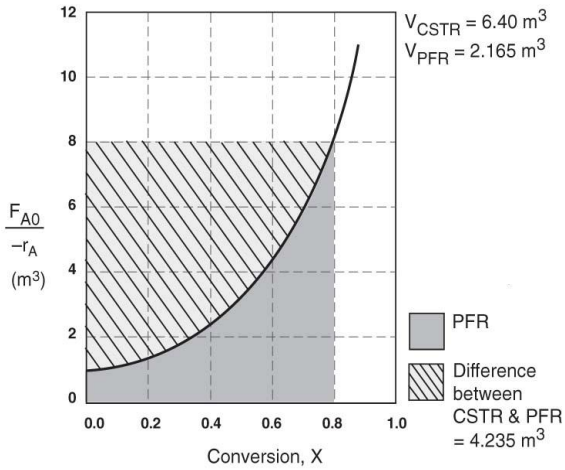
$$V = \left(\frac{F_{A0}}{-r_A}\right)X$$

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



43

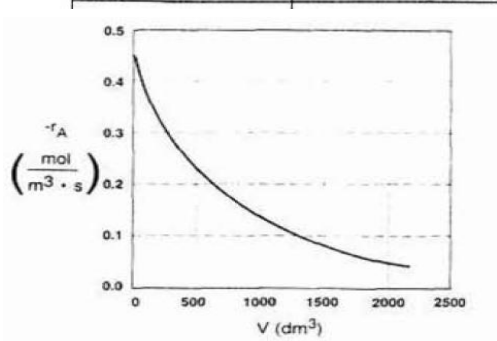
Graphically compare the volumes of a CSTR & PFR required for the same job (X=80%).

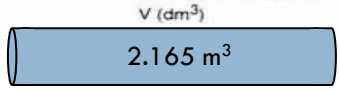


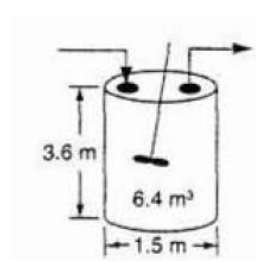
- For isothermal rxns greater than zero order, usually $V_{CSTR} > V_{PFR}$ for the same X and rxn conditions (T, F_i, etc.). Why?

44

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{mol}{m^3 \cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05







Inside the PFR:

X: 0.0–0.8

$-r_A$ = 0.45 – 0.05 mol/m^3·s

Inside the CSTR:

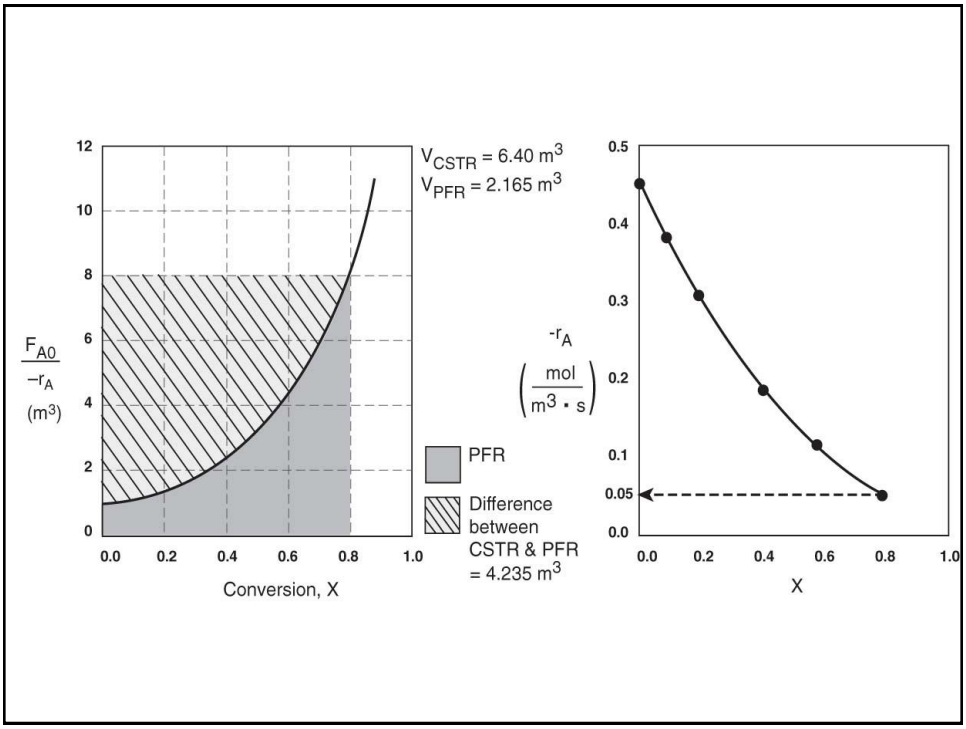
X: 0.8

$-r_A$ = 0.05 mol/m^3·s

45

بدر، هل تعلم أن أي ظاهرة
في المفاعل يمكن تفسيرها
بالريأكشن ريت!
صح والله؟
أنيس وبدر
123
افتح يا سمسم

47


V_{CSTR} = 6.40 m^3
V_{PFR} = 2.165 m^3
$\frac{F_{A0}}{-r_A}$ (m^3)
Conversion, X
PFR
Difference between CSTR & PFR = 4.235 m^3
$-r_A$ $\left(\frac{mol}{m^3 \cdot s}\right)$
X

51

Example 2-4 Comparing CSTR and PFR Sizes

- For isothermal reactions greater than zero order, the CSTR V will usually be greater than the PFR V for the same X and reaction conditions (T, F_i, etc.).
- That is because the CSTR is always operating at the lowest concentration and rxn rate.
- The PFR on the other hand starts at a high concentration and rate at the entrance and gradually decreases to the lowest values at the exit.
- Thereby, PFR requires less V because the volume is inversely proportional to the rate.
- However, for autocatalytic rxns, product-inhibited rxns, and nonisothermal exothermic reactions, these trends will not always be the case, as can be seen Chapters 7 and 8.

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Lecture 8

- Reactors in Series
  - CSTRs in series
  - PFRs in series

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2.5 Reactors in Series

- Note the streams and reactor labeling.
- Express the conversion achieved by/inside reactor 3 symbolically ($X|_{R3}$).

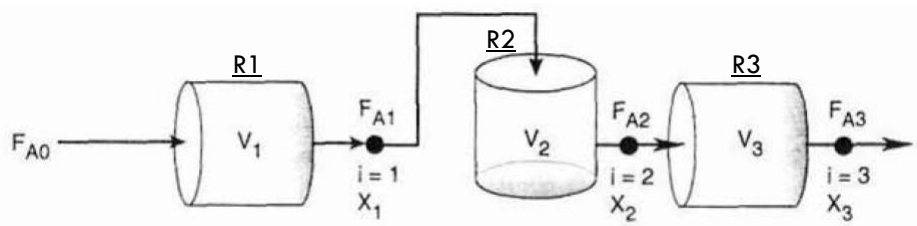

Figure 2-3 Reactors in series.

54

2.5 Reactors in Series

- Many times, reactors are connected in series so that the exit stream of one reactor is the feed stream for another reactor.
- For such cases, to speed calculations, conversion is defined in a new way (X_i):
- X_i is the conversion achieved up to point i with respect to F_{A0}.

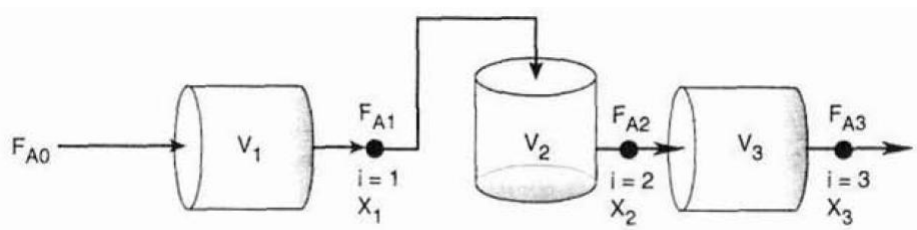

Figure 2-3 Reactors in series.

55

2.5 Reactors in Series

- Many times, reactors are connected in series so that the exit stream of one reactor is the feed stream for another reactor.
- X_i is defined as

$$X_i = \frac{\text{total moles of A reacted up to point } i}{\text{moles of A fed to the first reactor}} = \frac{F_{A0} - F_{Ai}}{F_{A0}}$$

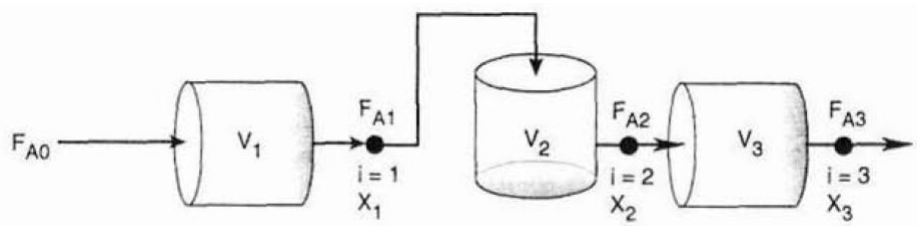

Figure 2-3 Reactors in series.

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- Express the conversion achieved up to point/stream 3 symbolically (X_3).
- X_3 is the total conversion achieved by all the three reactors.
- Since reactor 3 is the last reactor, X_3 is also known as the overall conversion.

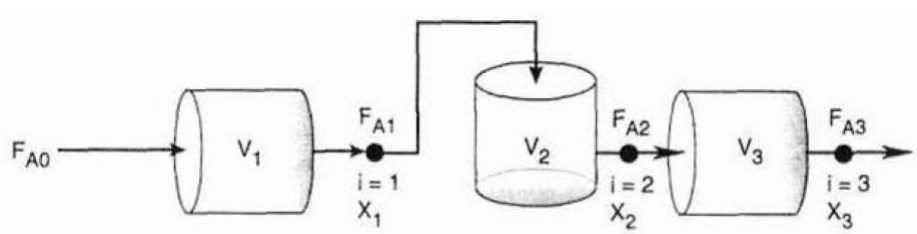

Figure 2-3 Reactors in series.

57

2.5 Reactors in Series

- Many times, reactors are connected in series so that the exit stream of one reactor is the feed stream for another reactor.
- X_i is defined as

$$X_i = \frac{\text{total moles of A reacted up to point } i}{\text{moles of A fed to the first reactor}} = \frac{F_{A0} - F_{Ai}}{F_{A0}}$$

$$\therefore F_{Ai} = F_{A0}(1 - X_i)$$

58

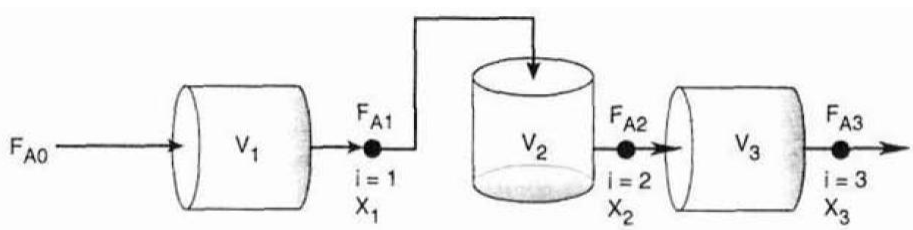

Figure 2-3 Reactors in series.

$$X_i = \frac{\text{total moles of A reacted up to point } i}{\text{moles of A fed to the first reactor}} = \frac{F_{A0} - F_{Ai}}{F_{A0}}$$

$$\therefore F_{Ai} = F_{A0}(1 - X_i)$$

Reactors in Series with no Side Streams

- Caution: this definition can only be used when the feed stream only enters the first reactor in the series and there are no side streams either fed or withdrawn.

59

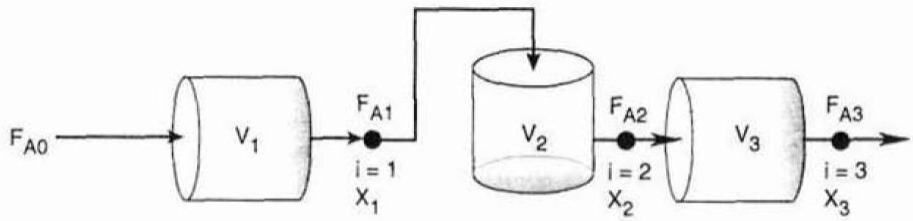

Figure 2-3 Reactors in series.

Let's consider three different schemes of reactors in series:

1. Two CSTRS
2. Two PFRs
3. A combination of PFRs & CSTRs in series.

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2.5.1 CSTRs in Series

10 min

Starting from the GMBE, derive the design equation for each of the shown reactors in terms of conversion:

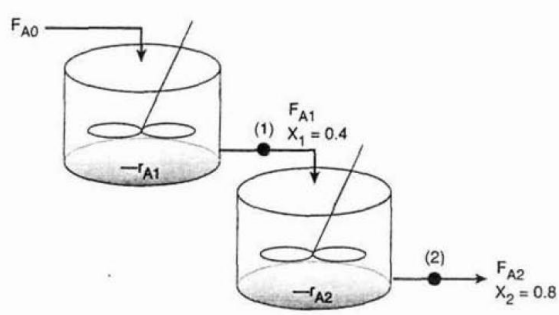

Figure 2-4 Two CSTRs in series.

$$F_{Ai} = F_{A0}(1 - X_i)$$

61

2.5.1 CSTRs in Series

Starting from the GMBE, derive the design equation for each of the shown reactors in terms of conversion:

- Reactor 1:

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

- Reactor 2:

$$V_2 = \frac{F_{A0}}{-r_{A2}} (X_2 - X_1)$$

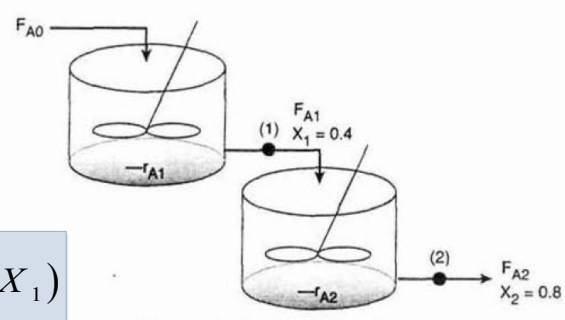

Figure 2-4 Two CSTRs in series.

Recall that: $-r_{A1}$ is evaluated at X_1 while $-r_{A2}$ is evaluated at X_2

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2.5.1 CSTRs in Series

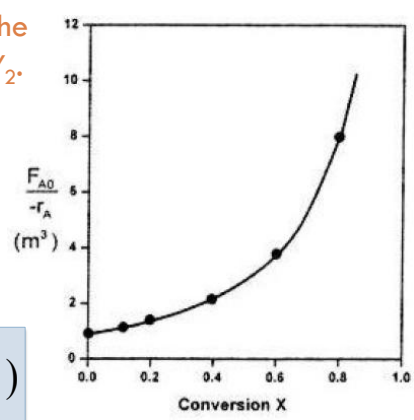
For X_1=0.4 & X_2=0.8, shade the areas that represent V_1 & V_2.

- Reactor 1:

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

- Reactor 2:

$$V_2 = \frac{F_{A0}}{-r_{A2}} (X_2 - X_1)$$



63

2.5.1 CSTRs in Series

For X_1=0.4 & X_2=0.8, shade the areas that represent V_1 & V_2.

- Reactor 1:

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

- Reactor 2:

$$V_2 = \frac{F_{A0}}{-r_{A2}} (X_2 - X_1)$$

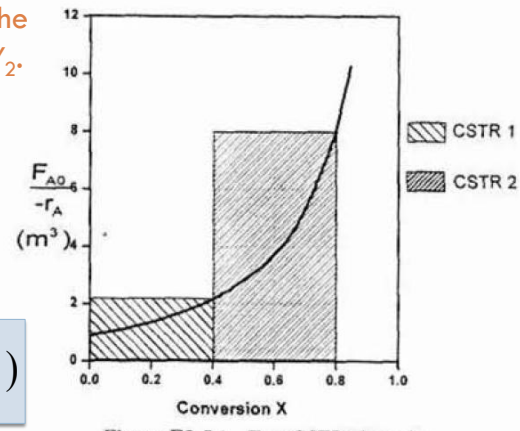


Figure E2-5.1 Two CSTRs in series.

Recall that: $-r_{A1}$ is evaluated at X_1 while $-r_{A2}$ is evaluated at X_2

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Example 2-5 Comparing Volumes of CSTRs in Series

20 min

For the two CSTRs in series, 40% conversion is achieved in the first reactor. What is the volume of each of the two reactors necessary to achieve 80% overall conversion of the entering species A.

$$V_1 = \frac{F_{A0}}{-r_{A1}} X_1 \qquad V_2 = \frac{F_{A0}}{-r_{A2}} (X_2 - X_1)$$

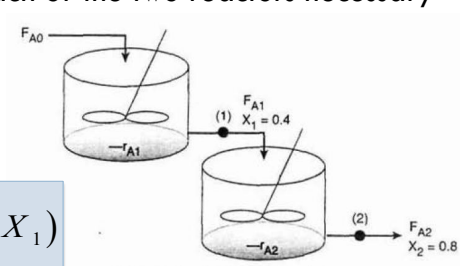


Figure 2-4 Two CSTRs in series.

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A]$(m³)	0.89	1.09	1.33	2.05	3.54	5.06	8.0

65

Example 2-5 Comparing Volumes of CSTRs in Series

V_1=0.82 m^3 , V_2=3.2 m^3

Why V_2 is larger than V_1?

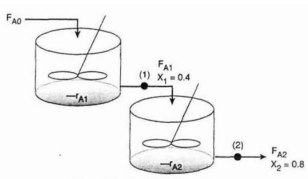
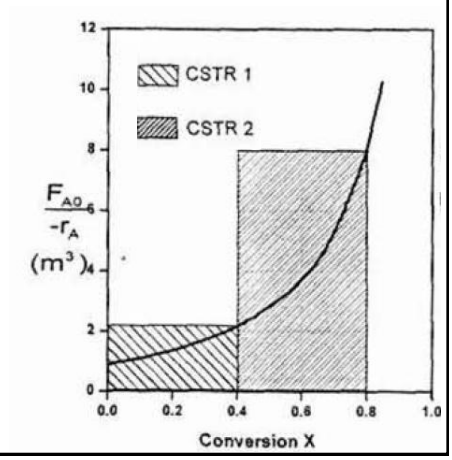


Figure 2-4 Two CSTRs in series.

X	0.0	0.4	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.195	0.05
$[F_{A0}/-r_A](\text{m}^3)$	0.89	2.05	8.0



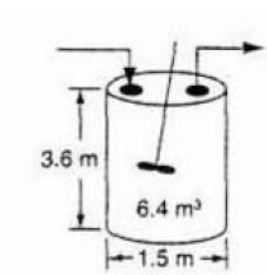
66

Example 2-5 Comparing Volumes of CSTRs in Series

V_1=0.82 m^3 , V_2=3.2 m^3 , so V_{tot} = V_1+V_2= 4.02 m^3

By comparison, V necessary to achieve X = 80% in one CSTR is:

$$V = \frac{F_{A0}}{-r_A}X = 8.0\times 0.8 = 6.4 \text{ m}^3$$



X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$[F_{A0}/-r_A](\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

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Example 2-5 Comparing Volumes of CSTRs in Series

V_1=0.82 m^3 , V_2=3.2 m^3 , $V = V_1+V_2$=4.02 m^3

By comparison, V necessary to achieve X = 80% in one CSTR is

V = 6.4 m^3

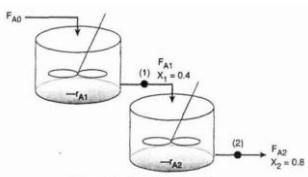
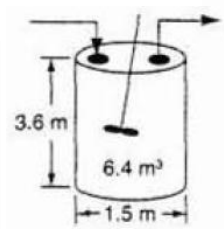
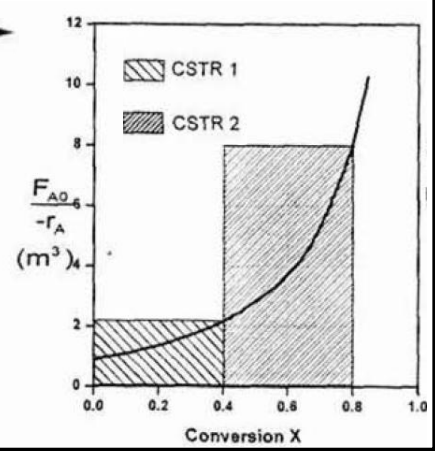


Figure 2-4 Two CSTRs in series.



X	0.0	0.4	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.195	0.05
$[F_{A0}/-r_A](\text{m}^3)$	0.89	2.05	8.0



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Example 2-5 Comparing Volumes of CSTRs in Series

V_1=0.82 m^3 , V_2=3.2 m^3 , $V = V_1+V_2$=4.02 m^3

By comparison, V necessary to achieve X = 80% in one CSTR is

V = 6.4 m^3

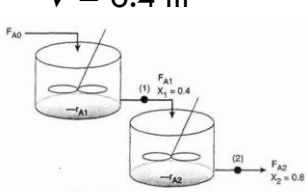
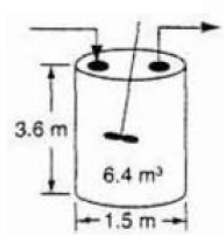
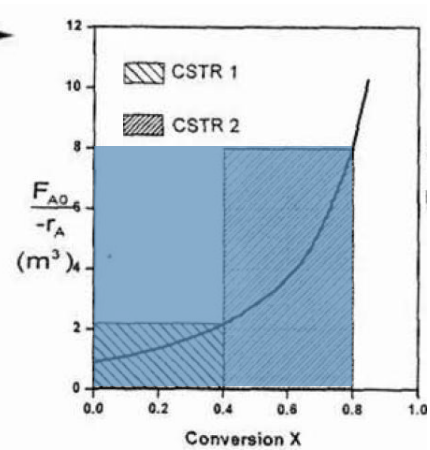


Figure 2-4 Two CSTRs in series.



X	0.0	0.4	0.8
$-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$	0.45	0.195	0.05
$[F_{A0}/-r_A](\text{m}^3)$	0.89	2.05	8.0



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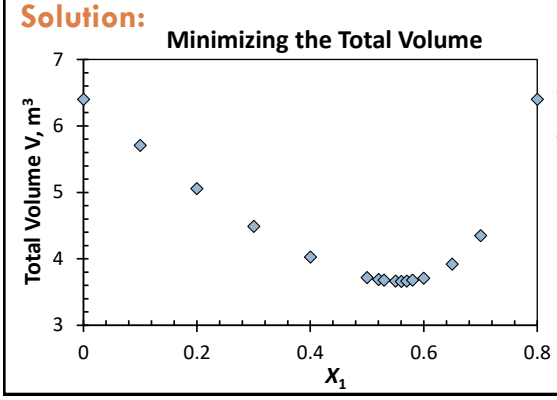
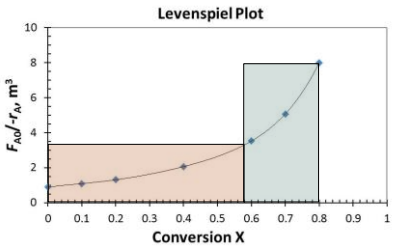
Example 2-5 Comparing Volumes of CSTRs in Series: optimizing the total volume (optional)

35 min

For example 2-5, determine the optimum value of the intermediate conversion (X_1) that minimizes the total volume of the reactors, keeping the overall conversion at 80%.

Solution:





Optimum $X_1 = 0.56$

V_1=1.75 m^3, V_2=1.92 m^3,

$V = V_1+V_2 = 3.66$ m^3

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Approximating a PFR by a large number of CSTRs in series

- Consider approximating a PFR with a number of small equal-volume CSTRs of V_i in series.
- We want to compare the total volume of all the five equally-sized CSTRs with the volume of one plug-flow reactor for the same conversion, say 80%.

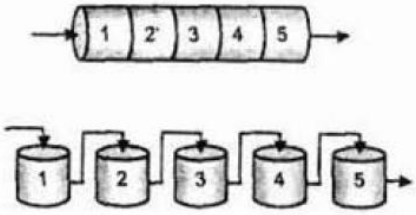

Figure 2-5 Modeling a PFR with CSTRs in series.

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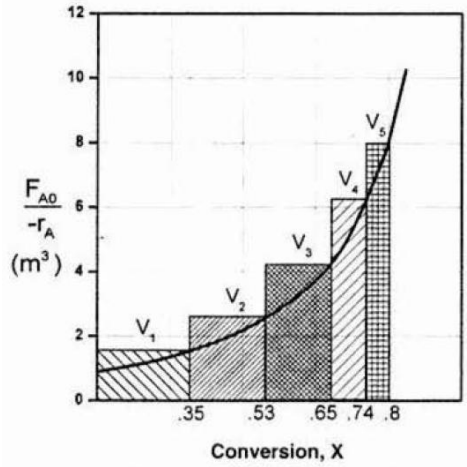


- Interesting observation!
- To achieve X = 80%,
  5 X V_i (CSTR) ≅ 1X V (PFR)
- As we make the *V* of each CSTR smaller and increase the no. of CSTRs, the total *V* of the CSTRs in series and the volume of the PFR will become identical.
- That is, we can model a PFR with a large number of CSTRs in series.

72

2.5.2 PFRs in Series

40 min

- We saw that two CSTRs in series gave a smaller total volume than a single CSTR to achieve the same *X*.
- Is this true for two PFRs connected in series?

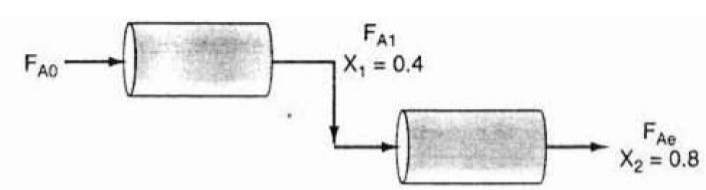
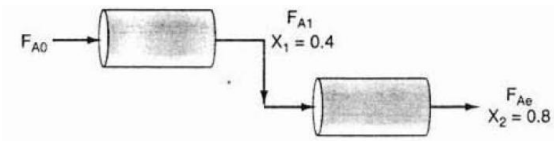


Figure 2-7 Two PFRs in series.

73

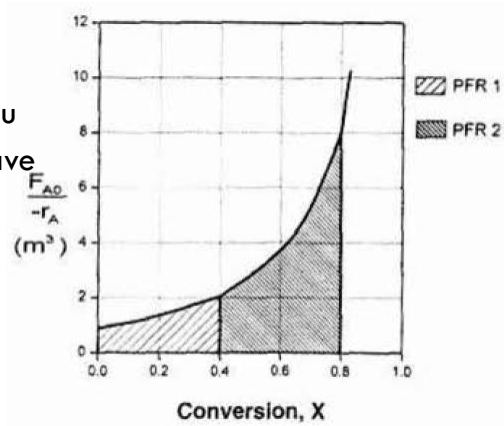
- Is that true for two PFRs connected in series?



$$V = \int_0^X \left(\frac{F_{A0}}{-r_A}\right) dX = \int_0^{X_2} \left(\frac{F_{A0}}{-r_A}\right) dX = \int_0^{X_1} \left(\frac{F_{A0}}{-r_A}\right) dX + \int_{X_1}^{X_2} \left(\frac{F_{A0}}{-r_A}\right) dX$$

$$\therefore V_{\text{single}} = \left[V_1 + V_2\right]_{\text{in series}}$$

- It does not matter whether you place two PFRs in series or have one PFR.
- The total reactor volume required to achieve the same conversion is identical.



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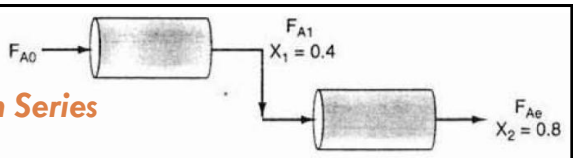


Example 2-6 Sizing PFRs in Series

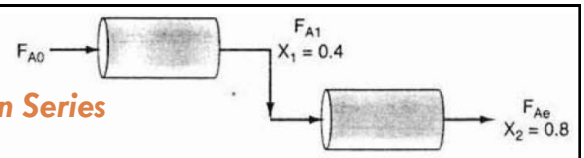
For the previously discussed rxn, calculate the reactor volumes V_1 & V_2 for the plug-flow sequence, shown above, when the intermediate X is 40% and the final X is 80%.

(F_{A0} = 0.4 mol/s)

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

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A]$(m³)	0.89	1.09	1.33	2.05	3.54	5.06	8.0

75



Example 2-6 Sizing PFRs in Series

2. *Simpson's one-third rule* (three-point) (Figure A-3).

$$V_1 = \int_0^{X1} \left(\frac{F_{A0}}{-r_A}\right) dX$$

$$\int_{X_0}^{X_2} f(X)\,dX = \frac{h}{3}[f(X_0) + 4f(X_1) + f(X_2)] \quad \text{(A-21)}$$

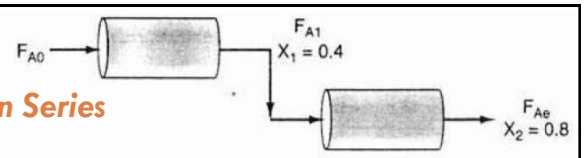
$$V_2 = \int_{X1}^{X2} \left(\frac{F_{A0}}{-r_A}\right) dX$$

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

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

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

76



Example 2-6 Sizing PFRs in Series

For the previously discussed rxn, calculate the reactor volumes V_1 & V_2 for the plug-flow sequence, shown above, when the intermediate X is 40% and the final X is 80%.

(F_{A0} = 0.4 mol/s)

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

Solution

V (m^3)	Num. Integ.	An. Integ.
V_1	0.551	0.549
V_2	1.614	1.598
V_{tot}	2.165	2.147
V (one PFR)	2.165	

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

78

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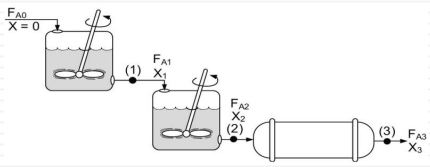
Lecture 9 – Week 3

- Combinations of CSTRs & PFRs in Series
- Space Time



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2.5.3 Combinations of CSTRs & PFRs in Series

- The final sequences we shall consider are combinations of CSTRs and PFRs in series.
- An industrial example:

  2 CSTR + PFR in series.
- This sequence is used to dimerize propylene into isohexenes.

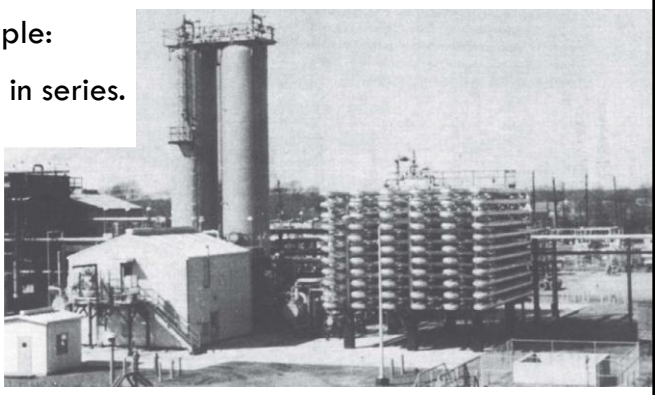

Figure 2-9 Dimersol G (an organometallic catalyst) unit (two CSTRs and one tubular reactor in series) to dimerize propylene into isohexanes. Institut Français du Pétrole process. [Photo courtesy of Editions Technip (Institut Français du Pétrole).]

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2.5.3 Combinations of CSTRs & PFRs in Series

- Example of dimerizing propylene into isohexenes:

$$2CH_3-CH=CH_2 \longrightarrow CH_3\overset{\overset{\displaystyle CH_3}{|}}{C}=CH-CH_2-CH_3$$

- A schematic of the industrial reactor system:

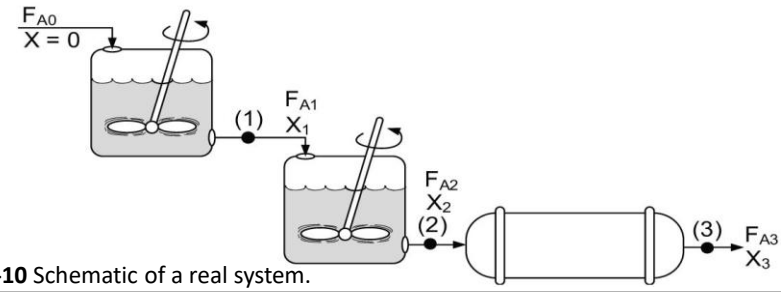
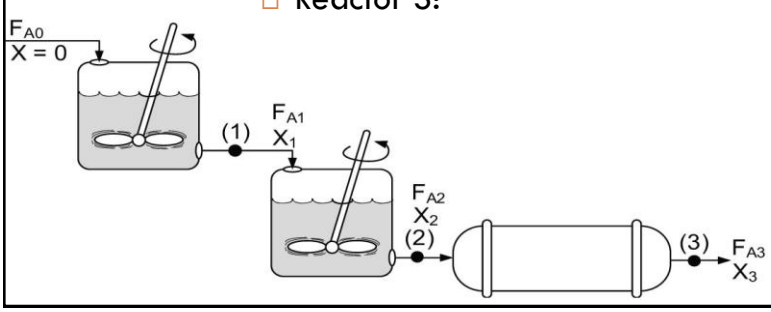


Figure 2-10 Schematic of a real system.

81

Write the design equation for each reactor in the shown reactor system:

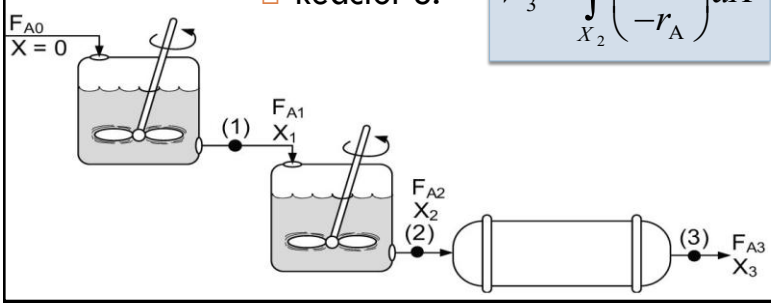
- Reactor 1:
- Reactor 2:
- Reactor 3:



82

Write the design equation for each reactor in the shown reactor system:

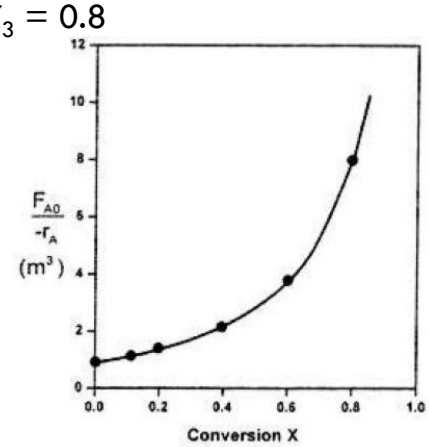
- Reactor 1: $$V_1 = \frac{F_{A0}}{-r_{A1}} X_1$$
- Reactor 2: $$V_2 = \frac{F_{A0}}{-r_{A2}} (X_2 - X_1)$$
- Reactor 3: $$V_3 = \int_{X_2}^{X_3} \left(\frac{F_{A0}}{-r_A} \right) dX$$

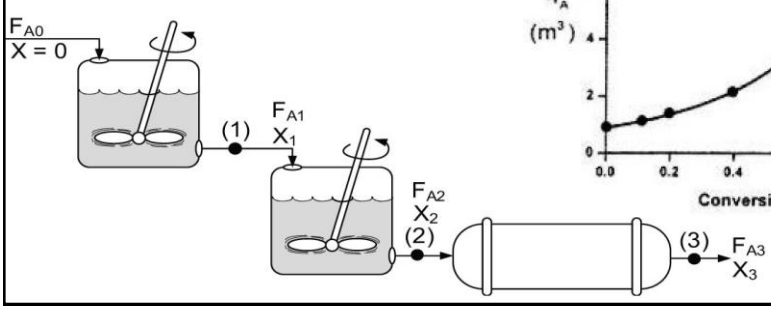


83

Assume that the presented dimerization rxn follows the same kinetics as that of the previously discussed isomerisation rxn.

Shade the area in the Levenspiel Plot that would give the volume of each of the shown reactors that are responsible to achieve $X_1 = 0.4$, $X_2 = 0.6$, & $X_3 = 0.8$

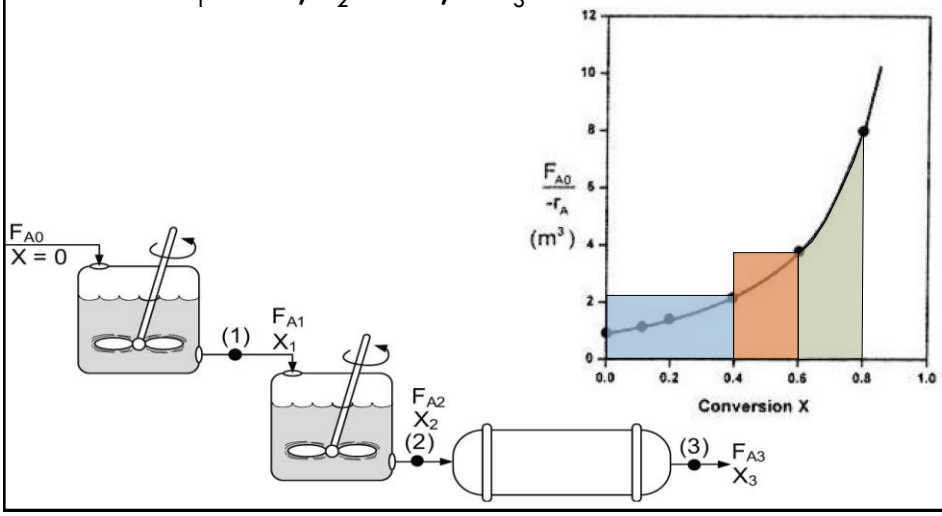




84

Assume that the presented dimerization rxn follows the same kinetics as that of the previously discussed isomerisation rxn.

Shade the area in the Levenspiel Plot that would give the volume of each of the shown reactors that are responsible to achieve $X_1 = 0.4$, $X_2 = 0.6$, & $X_3 = 0.8$



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2.5.3 Combinations of CSTRs & PFRs in Series

- The $-r_A$ vs. X data and the Levenspiel plots we have been using in the previous examples are typical of those found in isothermal reaction systems.

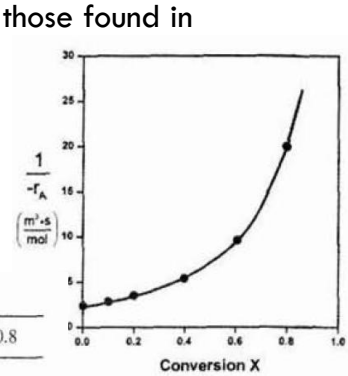

TABLE 2-2 PROCESSED DATA –I

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A\left(\frac{mol}{m^3 \cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05

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2.5.3 Combinations of CSTRs & PFRs in Series

- The $-r_A$ vs. X data and the Levenspiel plots we have been using in the previous examples are typical of those found in isothermal reaction systems.
- We will now consider a real reaction system that is carried out adiabatically.
- Isothermal reaction systems are discussed in Chapter 4 while adiabatic systems in Chapter 8.

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Example 2-7 An adiabatic Liquid-Phase Isomerization

10 min

The isomerization of butane: $n\text{-}C_4H_{10} \rightleftharpoons i\text{-}C_4H_{10}$ was carried out adiabatically in the liquid phase and the following data were obtained:

X	0.0	0.2	0.4	0.6	0.65
$-r_A$(kmol/m^3 · h)	39	53	59	38	25

Notes:

1. This is a real data for a real rxn that was carried out adiabatically.
2. $-r_A$ behaves differently compared to $-r_A$ of isothermal rxns.

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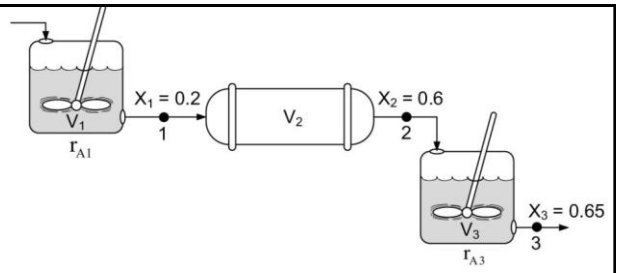


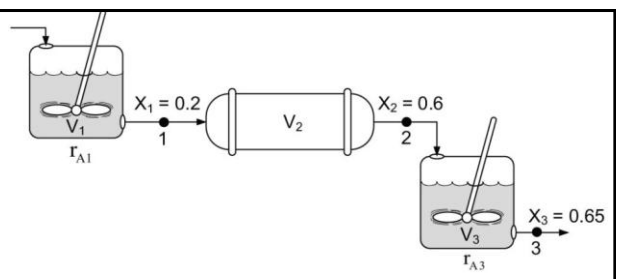
$$n\text{-}C_4H_{10} \rightleftharpoons i\text{-}C_4H_{10}$$

This rxn was carried out, on an industrial scale, adiabatically and in the liquid phase in the shown reactor scheme. For the specified conversions, calculate the volume of each of the reactors in this scheme. The entering molar flow rate of *n*-butane was fixed at 50 kmol/hr.

Solution:

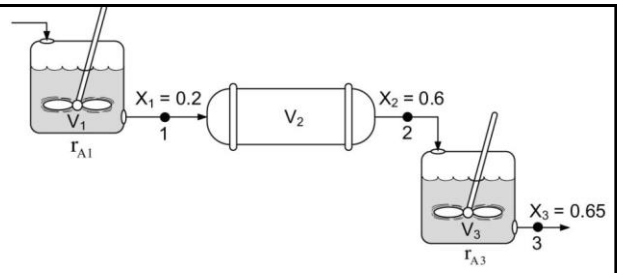
X	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m³ · h)	39	53	59	38	25
$[F_{A0}/-r_A]$ (m³)	1.28	0.94	0.85	1.32	2.0

89



X	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m³ · h)	39	53	59	38	25
$[F_{A0}/-r_A]$ (m³)	1.28	0.94	0.85	1.32	2.0

90



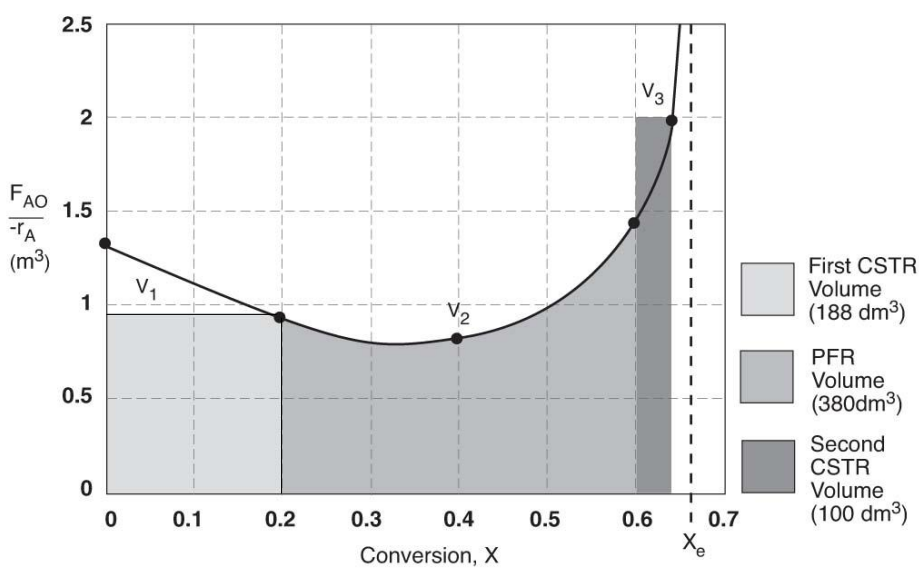
$$n\text{-}C_4H_{10} \rightleftharpoons i\text{-}C_4H_{10}$$

This rxn was carried out, on an industrial scale, adiabatically and in the liquid phase in the shown reactor scheme. For the specified conversions, calculate the volume of each of the reactors in this scheme. The entering molar flow rate of *n*-butane was fixed at 50 kmol/hr.

V (m³)	Value
V_1	0.188
V_2	0.380
V_3	0.100
V_{tot}	0.668

X	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m³ · h)	39	53	59	38	25
$[F_{A0}/-r_A]$ (m³)	1.28	0.94	0.85	1.32	2.0

91



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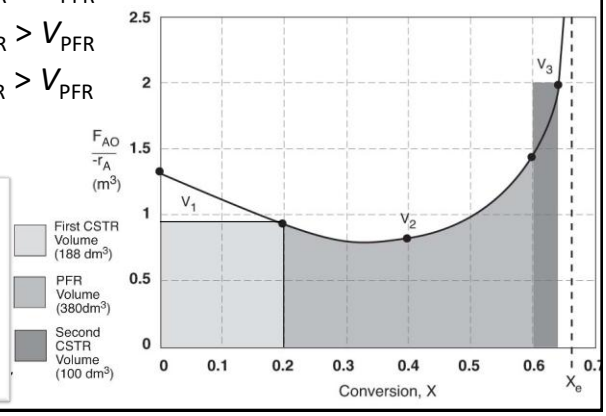
2.5.3 Comparing the CSTR and PFR Reactor Volumes and Reactor Sequencing

- Inspect the Levenspiel plot for the discussed adiabatic process.
- Compare the V_{CSTR} with V_{PFR} for the conversions:
  - $X=$ 0 to 0.2 , $V_{CSTR} < V_{PFR}$
  - $X=$ 0.2 to 0.6 , $V_{CSTR} > V_{PFR}$
  - $X=$0.6 to 0.65, $V_{CSTR} > V_{PFR}$

X	0.0	0.2
$-r_A$ (kmol/m^3 · h)	39	53
$[F_{A0}/-r_A]$ (m^3)	1.28	0.94



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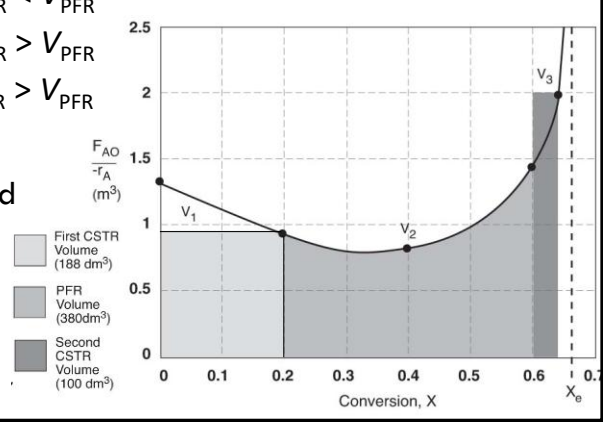
2.5.3 Comparing the CSTR and PFR Reactor Volumes and Reactor Sequencing

- Inspect the Levenspiel plot for the discussed adiabatic process.
- Compare the V_{CSTR} with V_{PFR} for the conversions:
  - $X=$ 0 to 0.2 , $V_{CSTR} < V_{PFR}$
  - $X=$ 0.2 to 0.6 , $V_{CSTR} > V_{PFR}$
  - $X=$0.6 to 0.65, $V_{CSTR} > V_{PFR}$
- Is there a better arrangement that would lead to a smaller V_{tot}?
- This will lead us to questions regarding *sequencing of reactors*.



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2.5.3 Comparing the CSTR and PFR Reactor Volumes and Reactor Sequencing

30 min

- In the *sequencing of reactors*, where the desired overall conversion is specified, one is often asked:

  "Which reactor should go first to minimize the no & total reactors' volume?"

- The answer is "**It Depends**!"
- It depends on the shape of the Levenspiel plot ($F_{A0}/-r_A$ vs. X) and on the relative reactor sizes.

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- In the *sequencing of reactors*, where the type, number, and volume of the reactors are specified, one is often asked:

  "Which reactor should go first to give the highest overall X ?"

- The answer is "**It Depends**!"
- It depends not only on the shape of the Levenspiel plots ($F_{A0}/-r_A$ vs. X), but also on the relative reactor sizes.
- Suppose you were given a Levenspiel plot & three reactors along with their volumes V_{CSTR1}=3 m^3, V_{CSTR2}= 2 m^3, & V_{PFR} = 1.2 m^3 and asked to find the highest possible conversion X.
- *What is No. possible arrangements?*

Permutation (تباديل) vs.
Combination (توافيق)

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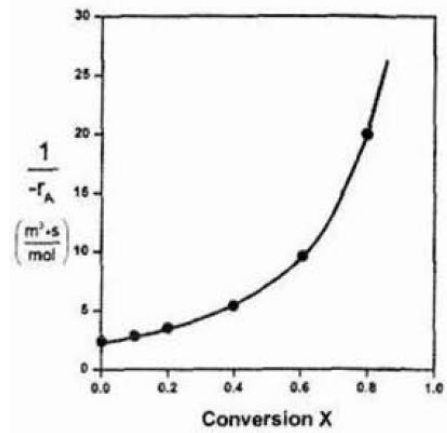
- Suppose you were given a Levenspiel plot & three reactors along with their volumes V_{CSTR1}=3 m^3, V_{CSTR2}= 2 m^3, & V_{PFR} = 1.2 m^3 and asked to find the highest possible conversion.
- *How would you calculate X?*



- The methods we used to calculate reactor volumes all apply, except the procedure is reversed and a trial-and-error solution is needed to find the exit overall *X* from each reactor.
- Example:

$$V = \frac{F_{A0}X}{-r_A\big|_{exit}}$$

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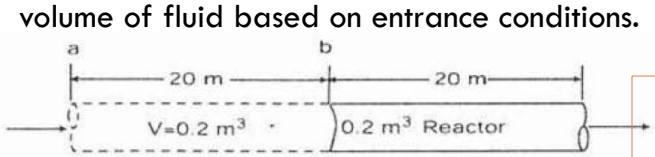
2.6 Some Further Definitions

40 min

2.6.1 Space Time

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

- The space time is the time necessary to process one reactor volume of fluid based on entrance conditions.



If υ_0 = 0.1 m^3/s, then τ = ?

Figure 2-12 Tubular reactor showing identical volume upstream.

- The time it takes for this fluid to enter the reactor completely is the space time.
- It is sometimes called the *holding time* or *mean residence time*.

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2.6.1 Space Time

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

- In the absence of dispersion (Chap. 14), the *space time* is equal to the *mean residence time* in the reactor, t_m, when $\upsilon = \upsilon_0$.
- This time is the average time the molecules spend in the reactor.

TABLE 2-4 TYPICAL SPACE TIME FOR INDUSTRIAL REACTORS[2]

Reactor Type	*Mean Residence Time Range*	*Production Capacity*
Batch	15 min to 20 h	Few kg/day to 100,000 tons/year
CSTR	10 min to 4 h	10 to 3,000,000 tons/year
Tubular	0.5 s to 1 h	50 to 5,000,000 tons/year

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Table 2-5 shows space times for six industrial reactions and reactors.

TABLE 2-5 SAMPLE INDUSTRIAL SPACE TIMES[3]

	Reaction	*Reactor*	*Temperature*	*Pressure atm*	*Space Time*
(1)	$C_2H_6 \rightarrow C_2H_4 + H_2$	PFR†	860°C	2	1 s
(2)	$CH_3CH_2OH + CH_3COOH \rightarrow CH_3CH_2COOCH_3 + H_2O$	CSTR	100°C	1	2 h
(3)	Catalytic cracking	PBR	490°C	20	$1\ s < \tau < 400\ s$
(4)	$C_6H_5CH_2CH_3 \rightarrow C_6H_5CH = CH_2 + H_2$	PBR	600°C	1	0.2 s
(5)	$CO + H_2O \rightarrow CO_2 + H_2$	PBR	300°C	26	4.5 s
(6)	$C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$	CSTR	50°C	1	20 min

†The reactor is tubular but the flow may or may not be ideal plug flow.

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Mean Residence Time (Optional)

- How is the mean residence time calculated for a flow reactor?
- Take the PFR as an example.
- Calculate the differential volume that each plug passes through in a differential amount of time:

$$dV = \upsilon \cdot dt$$

- Therefore, the average time necessary for a plug to travel from inlet to outlet of a tubular reactor (i.e. the mean residence time) is:

$$t = \int_0^V \frac{dV}{\upsilon}$$

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Lecture 10

- Space Velocity
- Tutorial

Prepared by: Dr Shaker Haji - CHENG 323

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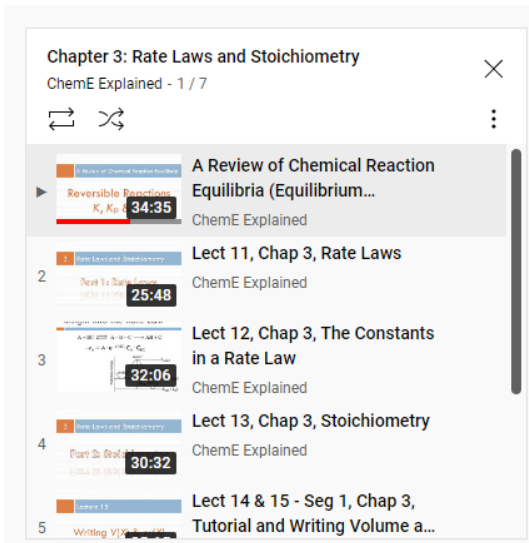
A Review on YouTube

Kindly watch the following video on YouTube (ChemE Explained) before next class:

A Review of Chemical Reaction Equilibria (Equilibrium Constants), Chap 3



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2.6 Some Further Definitions

2.6.1 Space Time

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

- The space time is the time necessary to process one reactor volume of fluid based on entrance conditions.

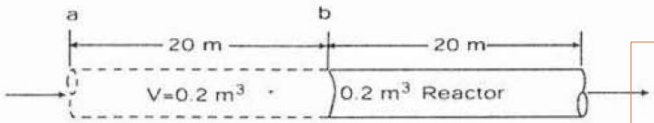

Figure 2-12 Tubular reactor showing identical volume upstream.

If $\upsilon_0 = 0.1\ m^3/s$, then $\tau = 2\ s$

- It is sometimes called the *holding time* or *mean residence time*.

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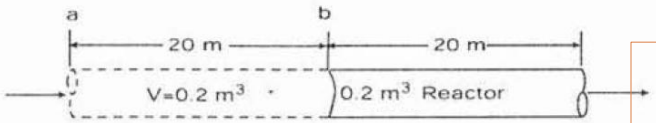
2.6.1 Space Velocity

$$SV \equiv \frac{\upsilon_0}{V}$$

- The space velocity indicates how many reactor volumes of feed can be treated in a unit time.



If $\upsilon_0 = 0.1\ m^3/s$, then SV = ?

Figure 2-12 Tubular reactor showing identical volume upstream.

- For the τ, the υ_0 is measured at the entrance conditions, but for the SV, other conditions are often used.

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2.6.1 Space Velocity

- The two SV commonly used in industry are the liquid-hourly space velocity (LHSV, h^{-1}) and gas-hourly space velocity (GHSV, h^{-1}).
- Why LHSV & GHSV are defined? Why not use the actual υ_0?
- Which gas stream has more quantity (moles)?

10^6 L/min (300 K, 2 atm) or 10^6 L/min (400 K, 3 atm)

1.8×10^6 L/min (STP) 2.0×10^6 L/min (STP)

$$LHSV \equiv \frac{\upsilon_0\big|_{liquid}}{V}$$

- Standard conditions are defined and used allow for easy and fair comparison.

$$GHSV \equiv \frac{\upsilon_0\big|_{STP}}{V}$$

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2.6.1 Space Velocity

- The υ_0 in the LHSV is frequently measured as that of a liquid feed rate at 60°F or 75°F, even though the feed to the reactor may be a vapor at some higher temperature.

υ_0 (gas)
@ actual T_0 & P_0

$$\text{LHSV} \equiv \frac{\upsilon_0\big|_{\text{liquid}}}{V}$$

$$\upsilon_0\,(\text{gas}) \xrightarrow{EOS} F_{T0}\,(\text{gas}) \xrightarrow{MM} \dot{m}_0\,(\text{gas}) = \dot{m}_0\,(\text{liquid}) \xrightarrow{\rho_{\text{liquid}}} \upsilon_0\,(\text{liquid})$$

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2.6.1 Space Velocity

- The gas volumetric flow rate, υ_0, in the GHSV is normally measured at STP.

υ_0 (gas)
@ actual T_0 & P_0

$$\text{GHSV} \equiv \frac{\upsilon_0\big|_{\text{STP}}}{V}$$

$$F_{T0}\,(\text{actual}) = F_{T0}\,(\text{STP})$$

(i.e., same quantity)

$$\frac{P_0 \times \upsilon_0}{T_0} = \frac{P_s \times \upsilon_0\big|_{\text{STP}}}{T_s}$$

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Example 2-8 Reactor Space Time and Velocity (Homework)

For the PFR reactor in Example 2-3 (2.165 m^3), calculate the space time and the GHSV where the entering volumetric flow rate (υ_0) was 2 L/s at 500 K and 830 kPa.

Answer:

1. τ = 18 min
2. GHSV = 15 h^{-1} (where $\mathrm{GHSV} \equiv \frac{\upsilon_0|_{\mathrm{STP}}}{V}$)

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Example 2-9 LHSV and WHSV Calculations (Optional)

On a laboratory scale, n-pentane was cracked at temperatures of 633-723 K and pressures of 10-60 bar using H-ZSM-5 catalyst.

For this reactive system, calculate the liquid hourly space velocity (LHSV) and the weight hourly space velocity (WHSV)

Additional information:

Catalyst: weight = 50 mg, bulk density = 720 g/L

Pentane: liquid flow rate = 0.5 mL/min, liquid density = 0.626 g/mL

Answer:

1. LHSV = 432 h^{-1} (where $\mathrm{LHSV} \equiv \frac{\upsilon_0|_{\mathrm{liquid}}}{V_{bed}}$)
2. WHSV = 375.6 h^{-1} (where $\mathrm{WHSV} \equiv \frac{\dot{m}_0}{m_{bed}}$)

Ref., DOI: https://doi.org/10.1039/C5NJ02733K

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Effect of increasing the SV on conversion

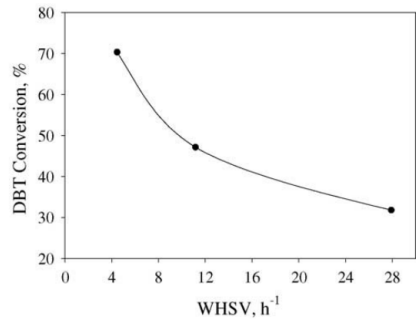

Fig. 12. The effect of WHSV on DBT conversion. Reaction conditions: $P = 1$ atm, $T = 310$ °C, $H_2/(n\text{-HD}) = 1.23$ molar ratio, and 0.58 wt.% Pt/Al_2O_3.

Shaker Haji et al. Hydrodesulfurization of model diesel using Pt/Al2O3 catalysts prepared by supercritical deposition. Catalysis Today, 99 (2005) 365–373.

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Note 1

Complete Suggested Problems #2

Note 2

Quiz #2

As announced

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- The previous examples show that if we know F_{i0} & the $-r_A$ vs. X data, then we can calculate the reactor V necessary to achieve a specified X.
- However, the r_A does not depend on X alone.
- It is also affected by the C_{i0}, T, P, & catalytic activity (for catalyzed rxns).
- So, the experimental data obtained in the lab and presented earlier as $-r_A$ vs. X are useful only in the design of full-scale reactors that are to be operated at the *identical conditions* as the lab experiments (C_{i0}, T, P, *catalyst*).
- However, such circumstances are **seldom** encountered.
- Therefore, we must revert to the methods that will be describe in Chap. 3 to obtain $-r_A$ as a function of X and other variables.

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Problem P2-5

20 min

You have a CSTR and a PFR each with a volume of 1.6 m^3. Use the given Levenspiel plot to calculate the X for each of the reactors in the following arrangement:

1. CSTR followed by PFR.
2. PFR followed by CSTR

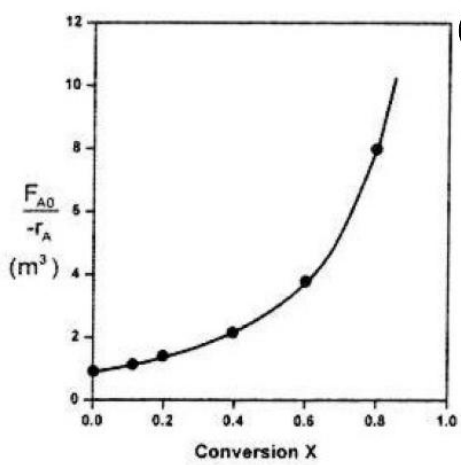

Figure 2-2 Levenspiel plot of processed data –2.

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

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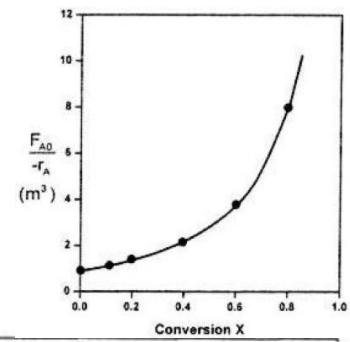
Problem P2-5

1. CSTR followed by PFR.



X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

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Problem P2-5

1. CSTR followed by PFR.

X	Value
CSTR X_1	0.54
PFR X_2	0.84

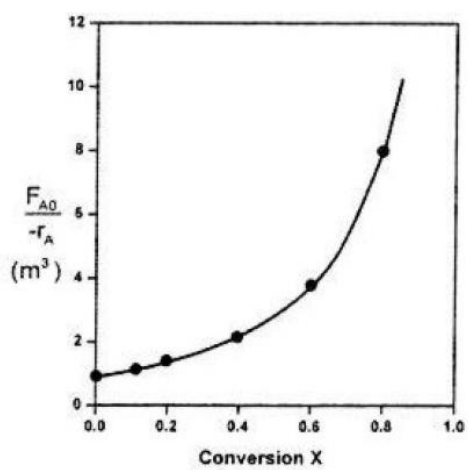

Figure 2-2 Levenspiel plot of processed data –2.

X	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$[F_{A0}/-r_A](m^3)$	0.89	1.09	1.33	2.05	3.54	5.06	8.0

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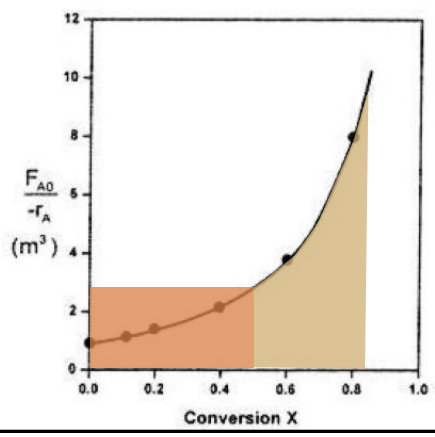
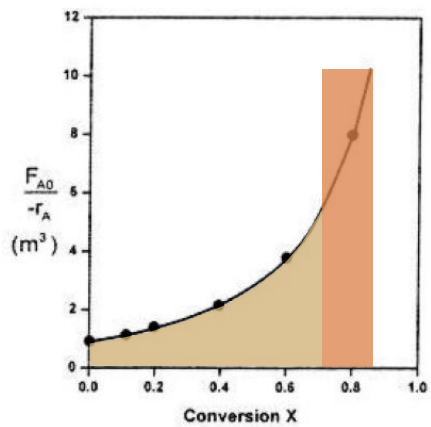
X	Value
CSTR X_1	0.541
PFR X_2	0.840

X	Value
PFR X_1	0.717
CSTR X_2	0.863

CSTR followed by PFR



PFR followed by CSTR



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In Summary

- We have seen that in the design of reactors that are to be operated at conditions (e.g., T & C_{i0}) identical to those at which the reaction rate data were obtained, we can size both CSTRs & PFRs alone or in various combinations.
- In principle, it may be possible to scale up a laboratory-bench or pilot-plant reaction system solely from knowledge of $-r_A$ as a function of X or C_A.
- However, for most reactor systems in industry, a scale-up process cannot be achieved in this manner because knowledge of $-r_A$ solely as a function of X is seldom, if ever, available under identical conditions.

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In Summary

- In Chapter 3, we shall see how we can obtain $-r_A = f(X)$ from information obtained either in the laboratory or from the literature.
- This relationship will be developed in a two-step process.
- In Step 1, we will find the rate law that gives the rate a function of concentration.
- In Step 2, we will find the concentrations as a function of X.
- Combining Steps I and 2 in Chapter 3, we obtain $-r_A = f(X)$.
- We can then use the methods developed in this chapter along with integral and numerical methods to size reactors.

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