

Chemical Reactor Design



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第2章

Conversion and Reactor Sizing

Chemical Reactor Design

化學反應裝置設計

Objectives

After completing Chapter 2, reader will be able to:

- ❁ Define conversion.
- ❁ 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 .

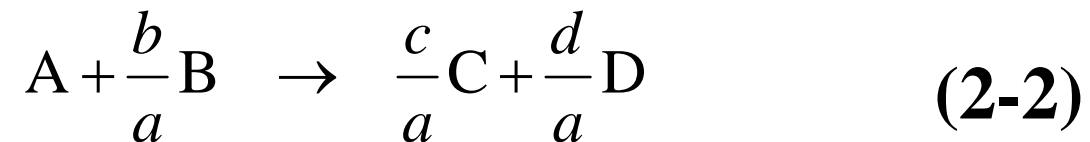
2.1 Definition of Conversion

Consider the general equation



Choose A as our *basis of calculation*

(The basis of calculation is most always the limiting reactant)



Questions

- How can we quantify how far a reaction has progressed ?
- How many moles of C are formed for every mole A consumed ?

The convenient way to answer these question is to define *conversion*.

$$X = \frac{\text{mole of A reacted}}{\text{mole of A fed}}$$

2.2 Batch Design Equations



In most batch reactors,

the longer a reactant is in the reactor, the more reactant is converted to product the reactant is exhausted. Consequently, in batch system, *the conversion X is a function of reaction time the reactants spend in the reactor.*

If N_{A0} is the number of moles of A initially in the reactor, then the total number of moles of A that have reacted after a time t is $[N_{A0} X]$

$$\begin{aligned} \left[\begin{array}{l} \text{mole of A} \\ \text{consumed} \end{array} \right] &= \left[\begin{array}{l} \text{mole of A} \\ \text{fed} \end{array} \right] \cdot \left[\frac{\text{moles of A reacted}}{\text{mole of A fed}} \right] \\ \left[\begin{array}{l} \text{mole of A} \\ \text{consumed} \end{array} \right] &= [N_{A0}] \cdot [X] \end{aligned} \quad (2-3)$$

The number of moles of A that remain in the reactor after a time t , N_A , can be expressed in terms of N_{A0} and X :

$$\begin{aligned} \left[\begin{array}{l} \text{moles of A} \\ \text{in reactor} \\ \text{at time } t \end{array} \right] &= \left[\begin{array}{l} \text{moles of A} \\ \text{initially fed to} \\ \text{reactor at } t = 0 \end{array} \right] - \left[\begin{array}{l} \text{moles of A that} \\ \text{have been consumed} \\ \text{by chemical reaction} \end{array} \right] \\ [N_A] &= [N_{A0}] - [N_{A0} X] \end{aligned} \quad (2-4)$$

2.2 Batch Design Equations

$$\frac{dN_A}{dt} = r_A V \quad (1-5)$$

The number of moles of A in the reactor after a conversion X

$$N_A = N_{A0} - N_{A0}X = N_{A0}(1 - X) \quad (2-4)$$

In term of conversion by differentiating equation

$$\frac{dN_A}{dt} = 0 - N_{A0} \frac{dX}{dt}$$

The design equation for a batch reactor in differential form is

The differential form
for a batch reactor

$$N_{A0} \frac{dX}{dt} = -r_A V \quad (2-5)$$

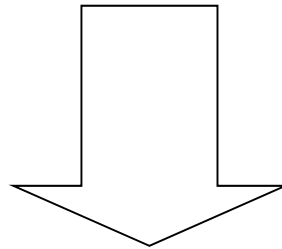
2.2 Batch Design Equations

The design equation for a batch reactor in differential form



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

(2-5)



**Write the mole balances
in terms of conversion**

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

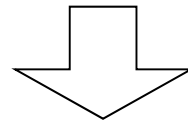
(2-6)

2.2 Batch Design Equations

The design equation for a batch reactor in differential form

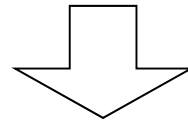


$$\frac{dN_A}{dt} = r_A V$$



Constant volume, $V = V_0$

$$\frac{1}{V} \frac{dN_A}{dt} = \frac{1}{V_0} \frac{dN_A}{dt} = \frac{d(N_A / V_0)}{dt} = \frac{dC_A}{dt} = r_A$$



$$r_A = \frac{dC_A}{dt}$$

(2-7)

2.2 Batch Design Equations

The design equation for a batch reactor in differential form



$$\frac{dN_A}{dt} = r_A V \quad (2-5)$$

$$N_{A0} \frac{dX}{dt} = -r_A V \quad (2-6)$$

The differential forms of the batch reactor mole balances, Eqs (2-5) and (2-6), are often used in the interpretation of reaction rate data (Chapter 5) and for reactors with heat effects (Chapter 9), respectively.

2.2 Batch Design Equations

- ❁ Batch reactors are frequently used in industry for both gas-phase and liquid-phase reactions.
- ❁ The lab bomb calorimeter reactor is widely used for obtaining reaction rate data.
- ❁ Liquid-phase reactions are frequently carried out in batch reactors when small-scale production is desired or operating difficulties rule out the use of continuous flow systems.



For constant-volume batch reactor, $V=V_0$

$$-\frac{1}{V_0} \frac{dN_A}{dt} = -\frac{d(N_A/V_0)}{dt} = -\frac{dC_A}{dt} = -r_A \quad C_A = \frac{N_A}{V_0}$$

For the most common batch reactors where volume is not predetermined function of time, the time necessary to achieve a conversion X is

The integral form
for a batch reactor

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



2.3 Design Equations for Flow Reactors

If F_{A0} is the molar flow rate of species A fed to a system at steady state, the molar rate at which species A is reacting within the entire system will be $F_{A0}X$.

$$[F_{A0}] \cdot [X] = \left[\frac{\text{moles of A fed}}{\text{time}} \right] \cdot \left[\frac{\text{moles of A reacted}}{\text{moles of A fed}} \right]$$

$$[F_{A0} \cdot X] = \left[\frac{\text{moles of A reacted}}{\text{time}} \right]$$



2.3 Design Equations for Flow Reactors

The molar flow rate

$$\begin{array}{c} \left[\begin{array}{l} \text{molar flow rate} \\ \text{at which A is} \\ \text{fed to the system} \end{array} \right] - \left[\begin{array}{l} \text{molar rate at which} \\ \text{consumed} \\ \text{within the system} \end{array} \right] = \left[\begin{array}{l} \text{molar flow rate} \\ \text{at which A} \\ \text{leaves the system} \end{array} \right] \\ [F_{A0}] - [F_{A0}X] = [F_A] \end{array}$$

Rearranging gives

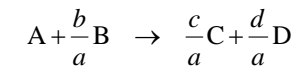
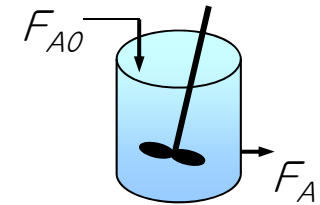
$$F_A = F_{A0}(1 - X) \quad (2-10)$$



2.3.1 CSTR or Backmix Reactor

- The design equation for a CSTR

$$V = \frac{F_{A0} - F_A}{-r_A} \quad (2-11)$$



- conversion of flow system

$$F_{A0} - F_A = F_{A0} X \quad (2-12)$$

- Combining (2-12) with (2-11)

$$V = \frac{F_{A0} X}{(-r_A)_{exit}} \quad (2-13)$$

*design equation
for a CSTR*

Equation to determine the CSTR volume necessary to achieve a specified conversion X . Since the exit composition from the reactor is identical to the composition inside the reactor, the rate of reaction is evaluated at the exit condition.

2.3.2 Tubular Flow Reactor (PFR)



- General mole balance equation

$$-\frac{dF_A}{dV} = -r_A \quad (1-12)$$

- conversion of flow system

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

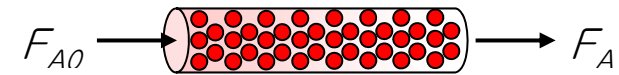
- The differential form of the design equation

$$F_{A0} \frac{dX}{dV} = -r_A \quad (2-15)$$

- Volume to achieve a specified conversion X

$$V = F_{A0} \int_0^X \frac{dX}{-r_A} \quad (2-16)$$

2.3.3 Packed-Bed Reactor (PBR)



- General mole balance equation

$$\frac{dF_A}{dW} = r_A' \quad (1-15)$$

- conversion of flow system

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

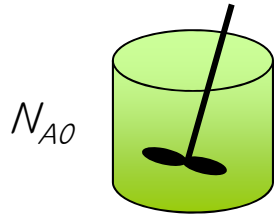
- The differential form of the design equation with $\Delta P \neq 0$

$$F_{A0} \frac{dX}{dW} = -r_A' \quad (2-17)$$

- The catalyst weight W to achieve a specified conversion X with $\Delta P=0$

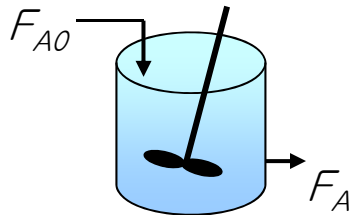
$$W = F_{A0} \int_0^X \frac{dX}{-r_A'} \quad (2-18)$$

Summary of Design Equation



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

Design equation
for a **batch reactor**



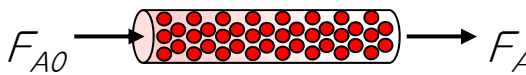
$$V = \frac{F_{A0} X}{(-r_A)_{exit}}$$

Design equation
for a **CSTR**



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

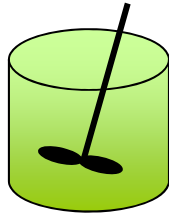
Design equation
for a **PFR**



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

Design equation
for a **PBR**

Summary of Design Equation



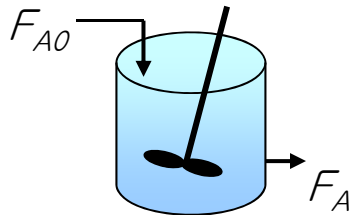
$$t = N_{A0} \int_0^{X(t)} \frac{dX}{-r_A V}$$

Reaction time

→ $\sim N_{A0}$

$\sim X$

$\sim 1/r_A V$



$$V = \frac{F_{A0} X}{(-r_A)_{exit}}$$

Reactor volume

(Catalyst weight)

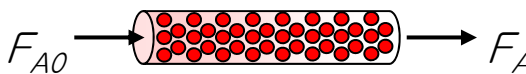


$$V = F_{A0} \int_0^X \frac{dX}{-r_A}$$

$\sim F_{A0}$

$\sim X$


$\sim 1/r_A'$



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

2.4 Applications of the design equation for continuous-flow reactor

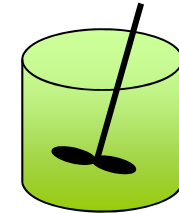
The rate of disappear of A, $-r_A$, is almost always a function of the concentrations of the various species present. When a single reaction is occurring, each of the concentrations can be expressed as a function of the conversion x ; consequently, $-r_A$, can be expressed as a function of X .


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

For a first-order reaction : $-r_A = kC_A = kC_{A0}(1 - X)$

How to use the raw data of chemical reaction rate?

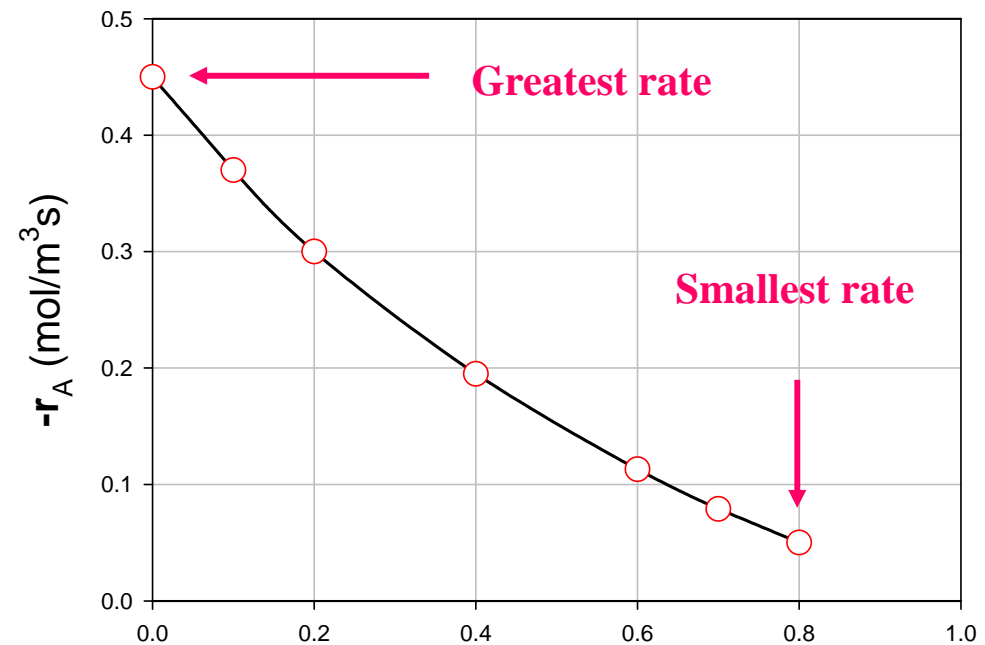
Consider the isothermal gas-phase isomerization



The laboratory measurements give the chemical reaction rate as a function of conversion.
(at $T=500\text{K}$, 8.2atm)

raw data

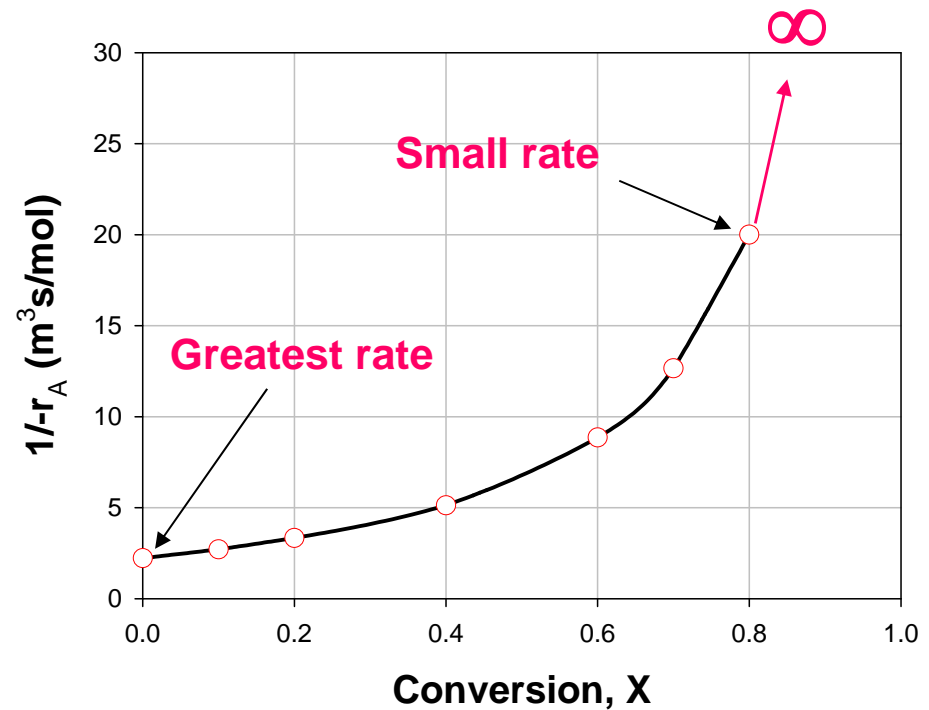
X	$-r_A$ (mol/m ³ s)
0.0	0.450
0.1	0.370
0.2	0.300
0.4	0.195
0.6	0.113
0.7	0.079
0.8	0.050



Levenspiel Plot

- rate data convert reciprocal rates, $1/-r_A$
- plot of $1/-r_A$ as a function of X

X	$-r_A$ (mol/m ³ s)	$1/-r_A$ (m ³ s/mol)
0.0	0.450	2,22
0.1	0.370	2,70
0.2	0.300	3,33
0.4	0.195	5,13
0.6	0.113	8,85
0.7	0.079	12,66
0.8	0.050	20,00

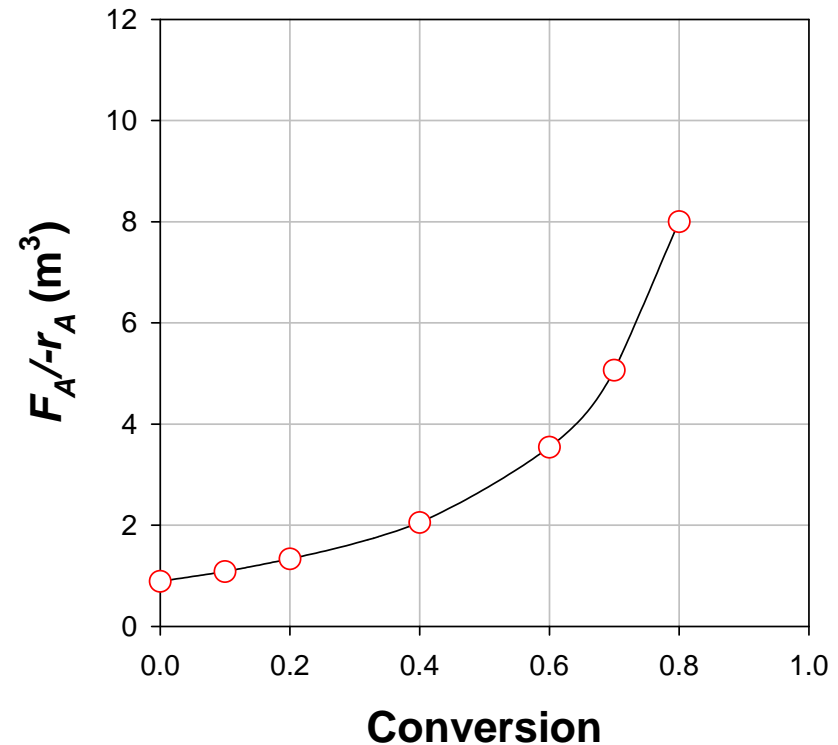


Levenspiel Plot

- plot of $[F_A / -r_A]$ as a function of $[X]$

Table 2-3

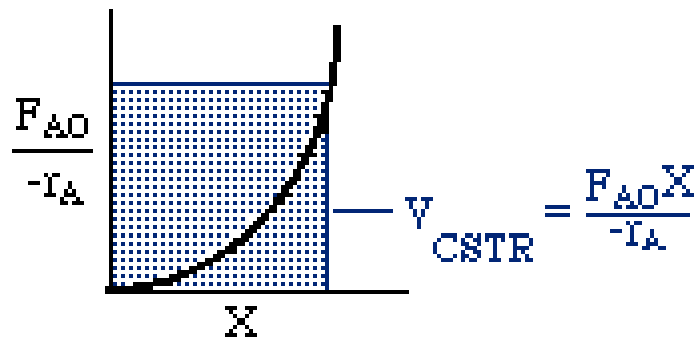
X	$-r_A$ (mol/m ³ s)	$1/-r_A$ (m ³ s/mol)	$F_A / -r_A$ (m ³)
0.0	0.450	2.22	0.89
0.1	0.370	2.70	1.08
0.2	0.300	3.33	1.33
0.4	0.195	5.13	2.05
0.6	0.113	8.85	3.54
0.7	0.079	12.66	5.06
0.8	0.050	20.00	8.00



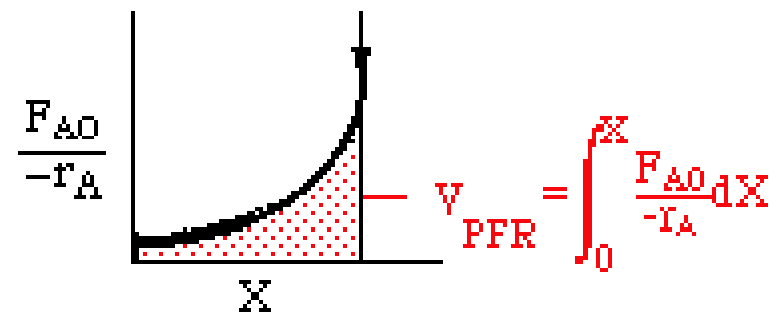
Reactor Size

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

CSTR



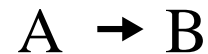
PFR



For $\frac{F_{A0}}{-r_A}$ vs. X , the volume of a CSTR and the volume of a PFR can be represented as the shaded areas in the Levenspiel plots.

Example 2-2 Sizing a CSTR

The reaction described by the data in Table 2-3 (below)



is to be carried out in a CSTR. Species A enters the reactor at a molar flow rate of 0.4 mol/s.

- (a) Using the data in Table 2-3, or Fig. 2-1, calculate the volume necessary to achieve 80% conversion in a CSTR.
- (b) Shade the area in Fig. 2-2 that would give the CSTR volume necessary to achieve 80% conversion.

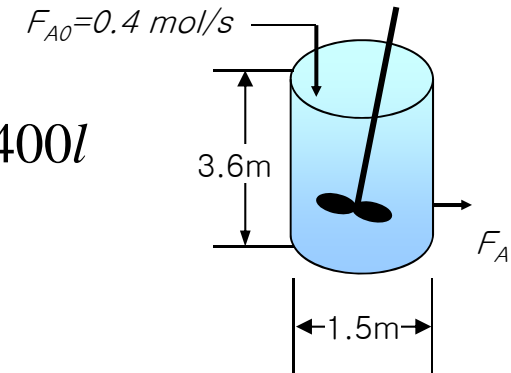
X	$-r_A$ (mol/m ³ s)	$1/r_A$ (m ³ s/mol)	F_A/r_A (m ³)
0.0	0.450	2.22	0.89
0.1	0.370	2.70	1.08
0.2	0.300	3.33	1.33
0.4	0.195	5.13	2.05
0.6	0.113	8.85	3.54
0.7	0.079	12.66	5.06
0.8	0.050	20.00	8.00

Table 2-3

Example 2-2 Sizing a CSTR

Calculate the volume necessary to achieve 80% conversion in a CSTR

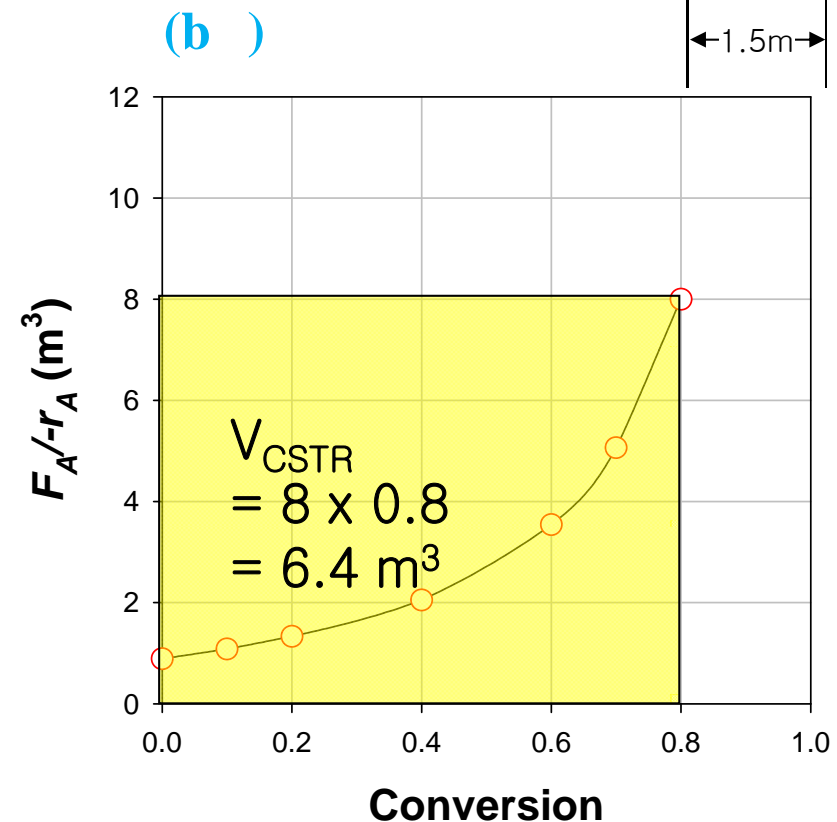
$$(a) \quad V = \frac{F_{A0}X}{(-r_A)_{exit}} = (0.4 \frac{\text{mol}}{\text{s}})(0.8)(20 \frac{\text{m}^3 \cdot \text{s}}{\text{mol}}) = 6.4 \text{m}^3 = 6400 \text{l}$$



X	$-r_A$ (mol/m ³ s)	$1/(-r_A)$ (m ³ s/mol)	$F_{A0}/(-r_A)$ (m ³)
0.0	0.450	2.22	0.89
0.1	0.370	2.70	1.08
0.2	0.300	3.33	1.33
0.4	0.195	5.13	2.05
0.6	0.113	8.85	3.54
0.7	0.079	12.66	5.06
0.8	0.050	20.00	8.00

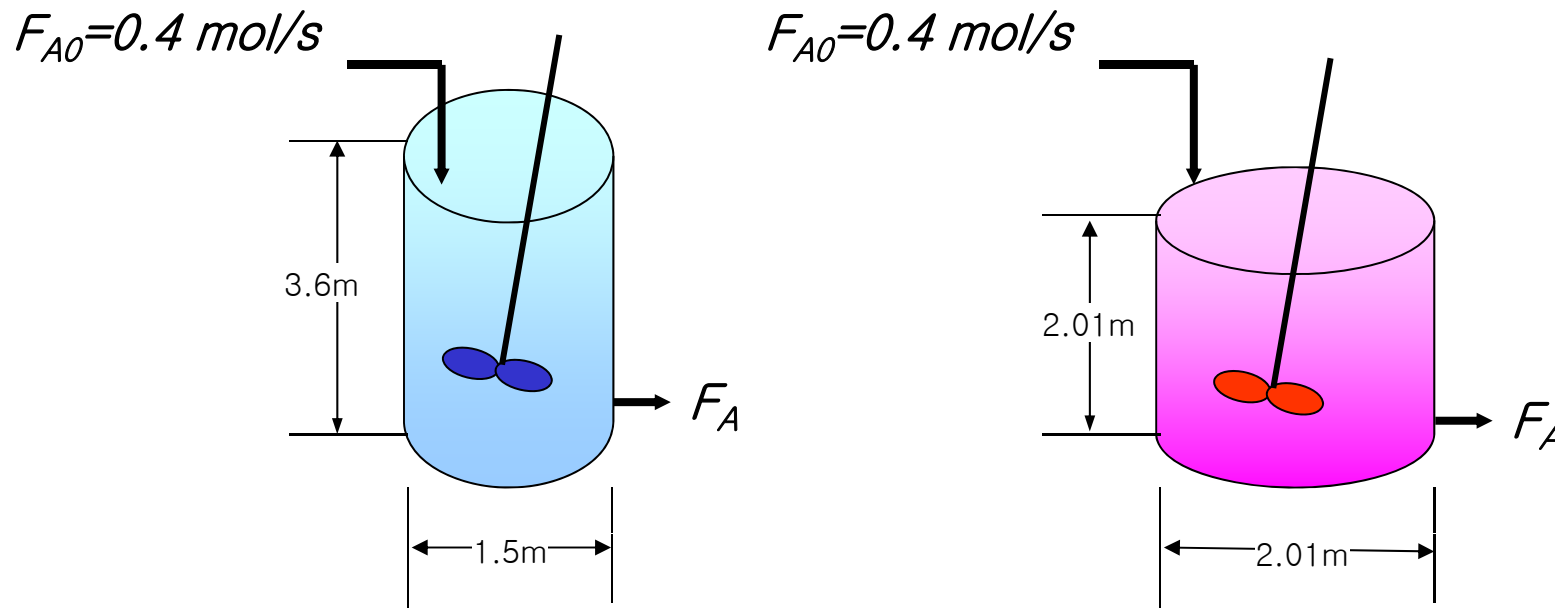
↑
EXIT

In CSTR, C, T, P, and X of the effluent stream are identical to that of the fluid within the reactor, because perfect mixing is assumed.



Example 2-2 Sizing a CSTR

The volume necessary to achieve 80% conversion in a CSTR is **6.4m³**.



It's a large CSTR, but this is a gas-phase reaction, and CSTRs are normally not used for gas-phase reaction, and CSTRs are used primarily for liquid-phase reactions.

Example 2-3 Sizing a PFR

Calculate the volume necessary to achieve 80% conversion in a PFR.

We shall use the *five point quadrature* formula (A-23) in Appendix A.4.

$$F_{A0} = 0.4 \text{ mol / s}$$

$$\begin{aligned}
 V &= \int_0^{X=0.8} \frac{F_{A0} dX}{-r_A} \\
 &= \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{2F_{A0}}{-r_A(X=0.4)} + \frac{4F_{A0}}{-r_A(X=0.6)} + \frac{F_{A0}}{-r_A(X=0.8)} \right] \\
 &= \left(\frac{0.2}{3} \right) [0.89 + 4(1.33) + 2(2.05) + 4(3.54) + (8.00)] m^3 = \left(\frac{0.2}{3} \right) (32.47 m^3) = 2.165 m^3
 \end{aligned}$$

X	$-r_A$ (mol/m ³ s)	$1/-r_A$ (m ³ s/mol)	$F_{A0}/-r_A$ (m ³)
0.0	0.450	2.22	0.89
0.1	0.370	2.70	1.08
0.2	0.300	3.33	1.33
0.4	0.195	5.13	2.05
0.6	0.113	8.85	3.54
0.7	0.079	12.66	5.06
0.8	0.050	20.00	8.00

$$\begin{aligned}
 V &= 2.165 \text{ m}^3 \\
 &= 2165 \text{ dm}^3
 \end{aligned}$$

Example 2-3 Sizing a PFR

Calculate the volume necessary to achieve 80% conversion in a PFR

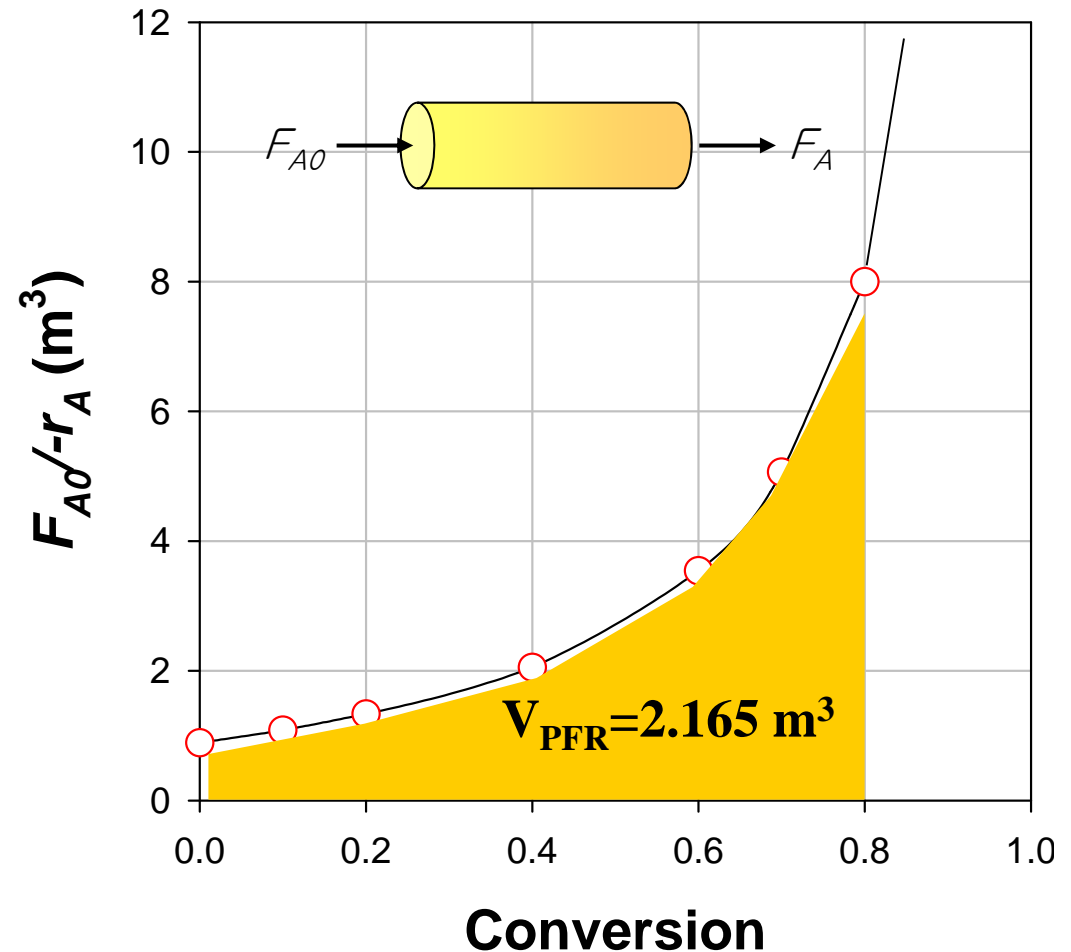
Graphic Method

$$V = \int_0^{X=0.8} \frac{F_{A0}}{-r_A} dX$$

= area under the curve
between $X=0$ and $X=0.8$

$$= 2165 \text{ dm}^3 (2.165 \text{ m}^3)$$

(see appropriate shaded area in Fig. E2-3.1)



Example 2-3 Sizing a PFR

Sketch the profile of $-r_A$ and X down the length of the reactor.

Solution



As we proceed down the reactor and more and more of reactant is consumed, the concentration of reactant decreases, as does the rate of disappearance of A. However, the conversion increases as more and more reactant is converted to product.

Simpson's rule (Appendix A.4 Eq. A-21)

$X=0.2, \Delta X=0.1$

$$\begin{aligned} V &= F_{A0} \int_0^{X=0.2} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.1)} + \frac{F_{A0}}{-r_A(X=0.2)} \right] \\ &= \left[\frac{0.1}{3} [0.89 + 4(1.08) + 1.33] \right] m^3 = \frac{0.1}{3} (6.54 m^3) = 0.218 m^3 = 218 dm^3 \end{aligned}$$

Example 2-3 Sizing a PFR

Sketch the profile of $-r_A$ and X down the length of the reactor.

Solution



Simpson's rule (Appendix A.4 Eq. A-21)

$X=0.4$, $\Delta X=0.2$

$$V = F_{A0} \int_0^{X=0.4} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.2)} + \frac{F_{A0}}{-r_A(X=0.4)} \right]$$
$$= \left[\frac{0.2}{3} [0.89 + 4(1.33) + 2.05] \right] m^3 = \frac{0.2}{3} (8.26 m^3) = 0.551 m^3 = 551 dm^3$$

Example 2-3 Sizing a PFR

Sketch the profile of $-r_A$ and X down the length of the reactor.

Solution



Simpson's rule (Appendix A.4 Eq. A-21)

$X=0.6$, $\Delta X=0.3$

$$V = F_{A0} \int_0^{X=0.6} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.3)} + \frac{F_{A0}}{-r_A(X=0.6)} \right]$$
$$= \left[\frac{0.3}{3} [0.89 + 4(1.625) + 3.54] \right] m^3 = \frac{0.3}{3} (10.93 m^3) = 1.093 m^3 = 1093 dm^3$$

Example 2-3 Sizing a PFR

Sketch the profile of $-r_A$ and X down the length of the reactor.

Solution



Simpson's rule (Appendix A.4 Eq. A-21)

$X=0.8$, $\Delta X=0.4$

$$V = F_{A0} \int_0^{X=0.8} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0)} + \frac{4F_{A0}}{-r_A(X=0.4)} + \frac{F_{A0}}{-r_A(X=0.8)} \right]$$
$$= \left[\frac{0.4}{3} [0.89 + 4(2.05) + 8.0] \right] m^3 = \frac{0.4}{3} (17.09 m^3) = 2.279 m^3 = 2279 dm^3$$

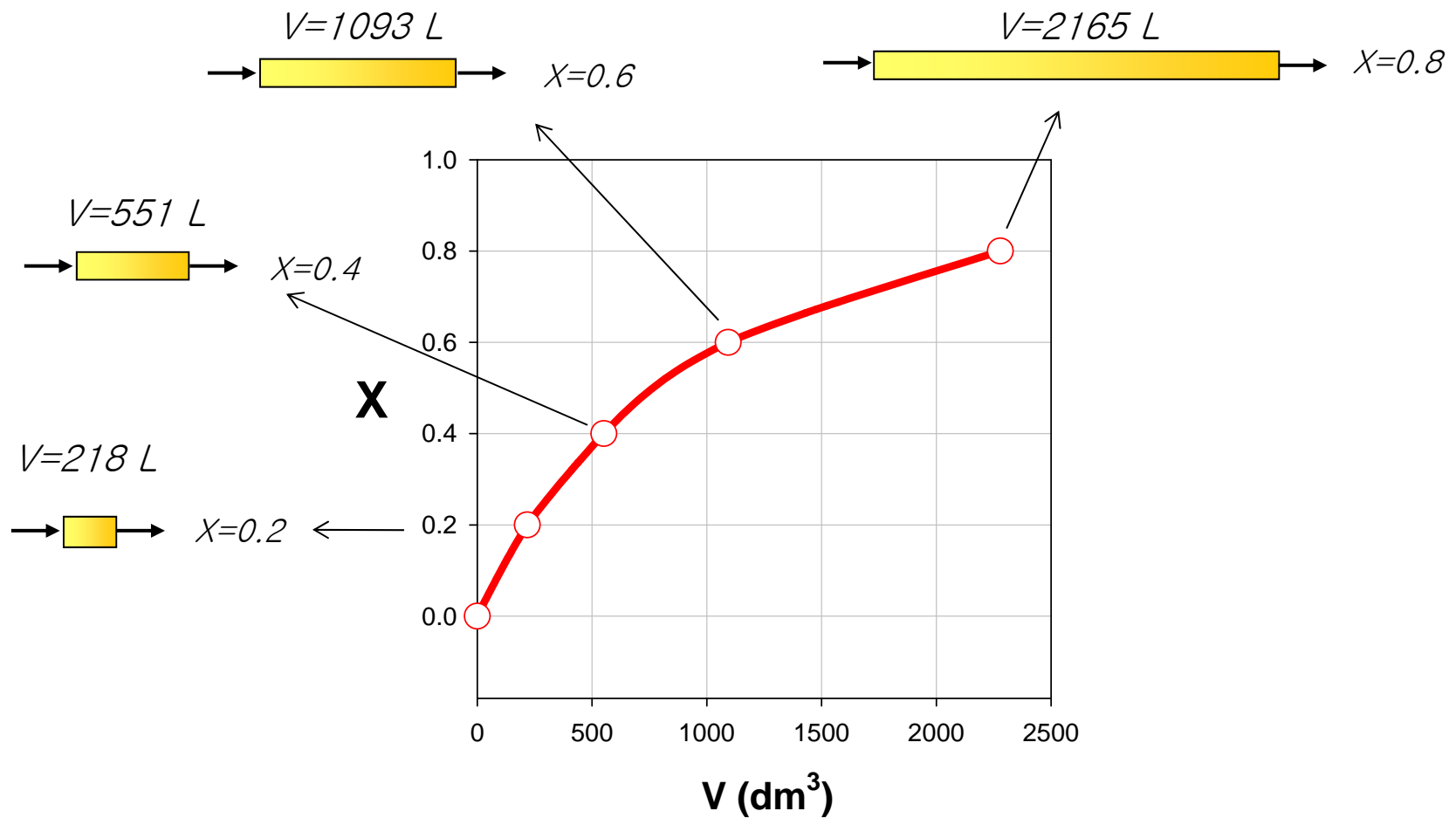
Example 2-3 Sizing a PFR

Sketch the profile of $-r_A$ and X down the length of the reactor.

X	0	0.2	0.4	0.6	0.8
$-r_A$ (mol/m³·s)	0.45	0.30	0.195	0.113	0.05
V (dm³)	0	218	551	1093	2279

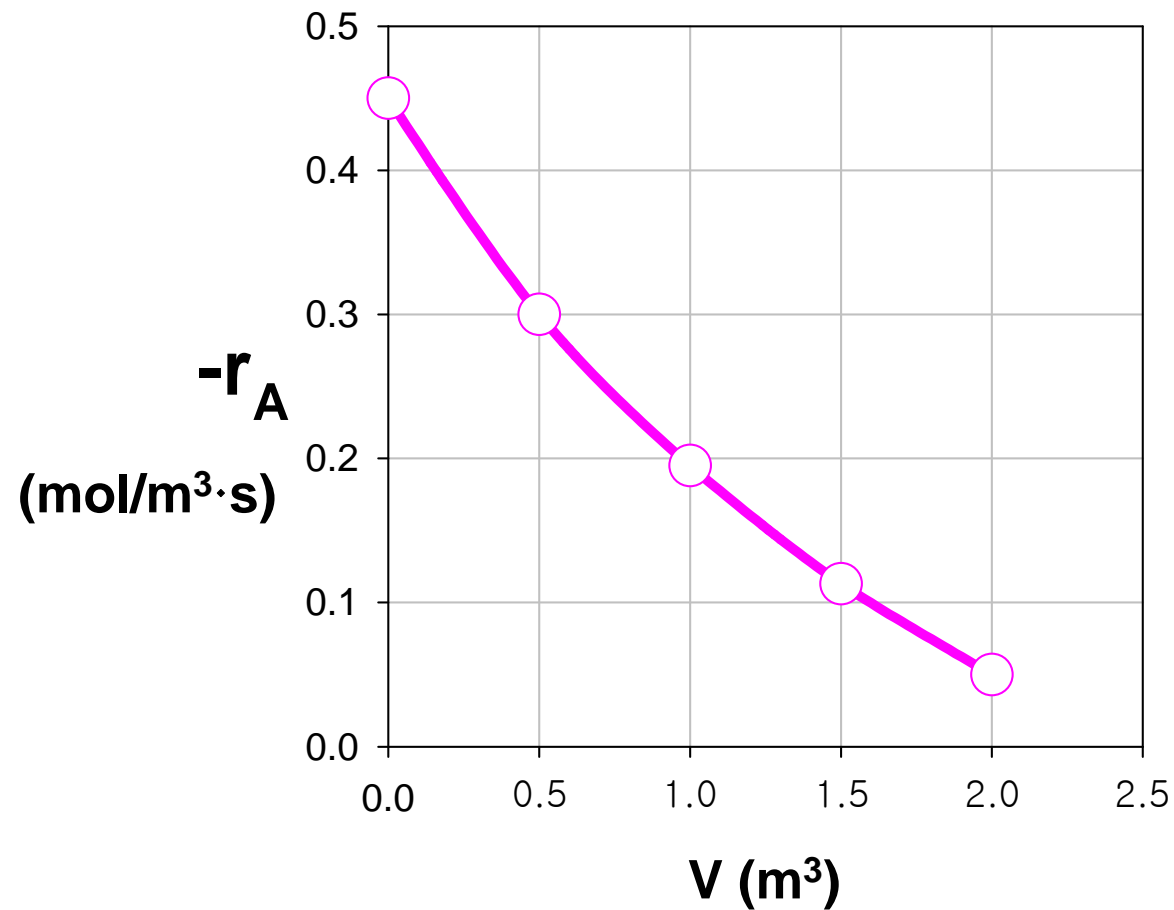
Example 2-3 Sizing a PFR

Sketch the profile of $-r_A$ and X down the length of the reactor.



Example 2-3 Sizing a PFR

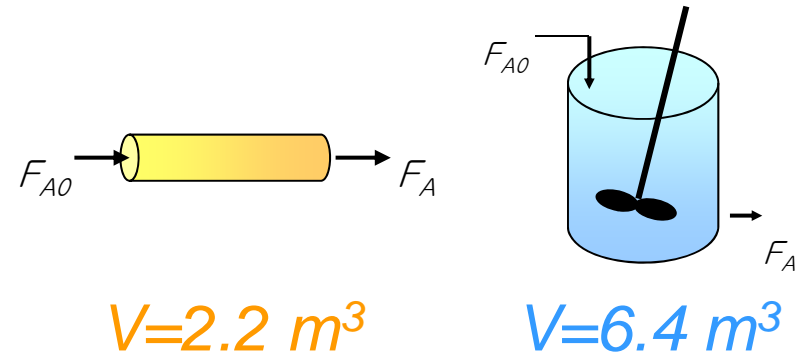
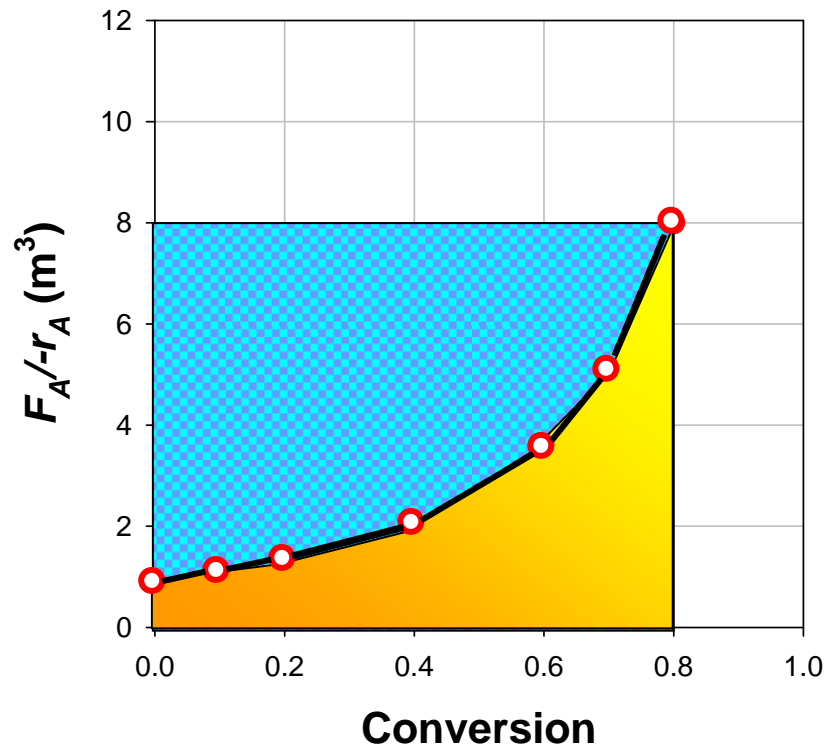
Sketch the profile of $-r_A$ and X down the length of the reactor.



Example 2-4 Comparing CSTR and PFR Sizes

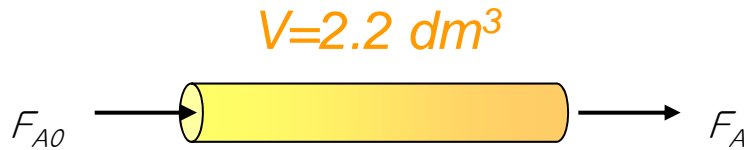
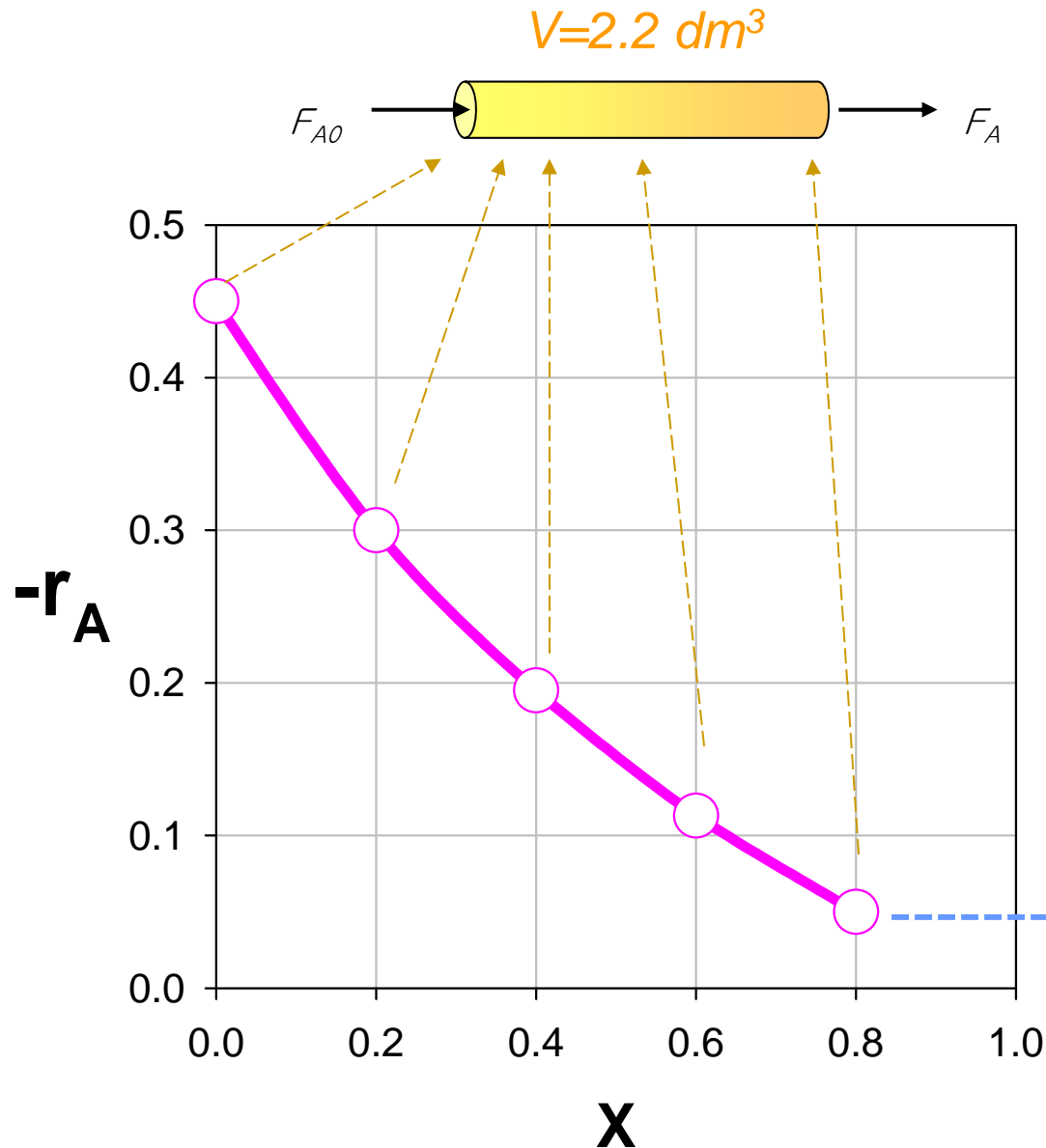
Calculate the volume necessary to achieve 80% conversion in a CSTR and a PFR

$$F_{A0} = 0.4 \text{ mol / s}$$



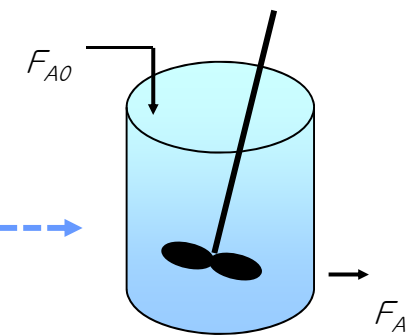
For **isothermal** reaction of greater than zero order, the PFR will always require a smaller volume than the CSTR to achieve.

Example 2-4 Comparing CSTR and PFR Sizes



The isothermal CSTR volume is usually greater than the PFR volume is that the CSTR is always operating at the lowest reaction rate ($-r_A=0.05$).

The PFR start at the higher rate at the entrance and gradually decreases to the exit rate, thereby requiring less volume because the volume is inversely proportional to the rate.



$V=6.4 \text{ dm}^3$

Laboratory and Full-scale operating conditions must be identical.

-If we know the molar flow rate to the reactor and the reaction rate as a function of conversion, then we can calculate the reactor volume necessary to achieve a specific conversion.

-However, the rate does not depend on conversion alone. It is also affected by the initial concentrations of the reactants, the temperature, and the pressure.

-Consequently, the experimental data obtained in the laboratory are useful only in the design of full-scale reactors that are to be operated at the same conditions as the laboratory experiments (T , P , C_{A0}).

-This conditional relationship is generally true; i.e., to use laboratory data directly for sizing reactors, the laboratory and full-scale operating conditions must be identical.

-Usually, such circumstances are seldom encountered and we must revert to the methods described in Chapter 3 to obtain $-r_A$ as a function of X .

To size flow reactor, only need $-r_A=f(X)$,

It is important to understand that

if the rate of reaction is available or can be obtained solely as a function of conversion, $-r_A=f(X)$, or

if it can be generated by some intermediate calculations,

one can design a variety of reactor or a combination of reactors.

In Chapter 3, we show how we obtain the relationship between reaction rate and conversion from rate law and reaction stoichiometry.

To summarize these last examples....

In the design of reactors that are to be operated at conditions (e.g., temperature and initial concentration) identical to those at which the reaction rate data were obtained, we can size (determine the reactor volume) both CSTRs and 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.

To summarize these last examples....

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 as a function of concentration and **in Step 2**, we will find the concentrations as a function of conversion. Combining Step 1 and 2 in Chapter 3, we obtain $-r_A=f(X)$.