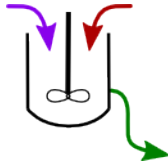


# Introduction to Reactor Design

## ChE 3K4



Kevin Dunn, 2013

(with credit to Dr. P. Mhaskar for many of the slides)

kevin.dunn@mcmaster.ca

<http://learnche.mcmaster.ca/3K4>

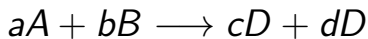
Overall revision number: 24 (January 2013)

## Chapter 2: Major ideas for this section

- A Definition of conversion
- B Reactor design *for a specified conversion*
- C Graphical interpretation/solution of CSTR and PFR design equations

# Conversion

Consider



Consider species  $A$  to be the **basis** (usually we pick the one which gets consumed to completion first, i.e. the limiting reagent).

Useful to express **extent of reaction** in terms of **conversion** of  $A$ :

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

To simplify notation, use  $X$  (without subscript).

# Conversion

## Remarks

- ▶ In a batch reactor,  $X$  is a *function of time*
  - ▶ For irreversible reaction,  $X \rightarrow 1$  as  $t \rightarrow \infty$
  - ▶ For reversible reaction,  $X \rightarrow X_e$  (equilibrium conversion) as  $t \rightarrow \infty$
  
- ▶ In flow reactors (CSTR and PFR) the  $X$  is a *function of volume*, which reflects the amount of time reactants spend in the reactor

# Design equations in terms of conversion

In this section we consider rewriting the previously derived equations from Chapter 1 (called the design equations) in terms of conversion.

We had previously used concentration  $C_A$  and molar flow  $F_A$ . Now we will use  $X$ , conversion.

We consider our 4 reactors (numbers refer to Fogler):

2.2 Batch

2.3.1 CSTR

2.3.2 PFR

2.3.3 PBR

# Batch systems

First express  $N_A$  in terms of  $X$

$$\begin{aligned} \left( \begin{array}{c} \text{moles } A \\ \text{reacted} \end{array} \right) &= \left( \begin{array}{c} \text{moles } A \\ \text{fed} \end{array} \right) \cdot \left( \frac{\text{moles } A \text{ reacted}}{\text{moles } A \text{ fed}} \right) \\ &= N_{A0} \cdot X \end{aligned}$$

$$\begin{aligned} \left( \begin{array}{c} \text{moles } A \text{ at} \\ \text{time } t \end{array} \right) &= \left( \begin{array}{c} \text{initial} \\ \text{moles } A \end{array} \right) - \left( \begin{array}{c} \text{moles } A \\ \text{consumed} \end{array} \right) \\ N_A &= N_{A0} - N_{A0} \cdot X \\ N_A &= N_{A0}(1 - X) \end{aligned}$$

# Batch systems

- ▶ Recall the mole balance equation (assumptions?):

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

- ▶ Integral form:

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

Design feature for batch systems: *time*

# Flow systems: CSTRs, PFRs and PBRs

$$F_{A0}X = \left( \frac{\text{moles } A \text{ fed}}{\text{time}} \right) \cdot \left( \frac{\text{moles } A \text{ reacted}}{\text{moles } A \text{ fed}} \right)$$

$$F_{A0}X = \frac{\text{moles } A \text{ reacted}}{\text{time}}$$

$$\left( \begin{array}{c} \text{molar rate of} \\ A \text{ leaving} \end{array} \right) = \left( \begin{array}{c} \text{molar rate} \\ \text{of } A \text{ fed} \end{array} \right) - \left( \begin{array}{c} \text{molar rate of} \\ A \text{ consumed} \end{array} \right)$$

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

$$F_A = F_{A0}(1 - X)$$

Draw a picture here →



# CSTR

- ▶ Recall the mole balance equation (what were the assumptions?):

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

$$V = \frac{F_{A0} - F_{A0}(1 - X)}{-r_A}$$

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

- ▶  $r_A$ : taken inside the reactor = exit conditions

Design feature for CSTR systems: *volume*

# PFR

Recall the mole balance equation (what were the assumptions?):

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

But  $F_A = F_{A0}(1 - X)$

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

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

Integral form:

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

Design feature for PFR systems: *volume*

# PBR

Follows a similar derivation:

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

Integral form:

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

Design feature for PBR systems: *catalyst weight*

## Summary so far Apply to a 1st order system

**Remark:** we generally obtain  $-r_A$  vs  $X$  from rate equation, e.g.  $-r_A = kC_A$ . Consider a flow reactor:

$$F_A = F_{A0}(1 - X)$$

$$C_A = \frac{F_A}{q} = \frac{F_{A0}(1 - X)}{q}$$

If  $q = q_0$  (under what conditions would this hold?):

$$C_A = \frac{F_{A0}}{q_0}(1 - X)$$

$$C_A = C_{A0}(1 - X)$$

and

$$-r_A = kC_A = kC_{A0}(1 - X)$$

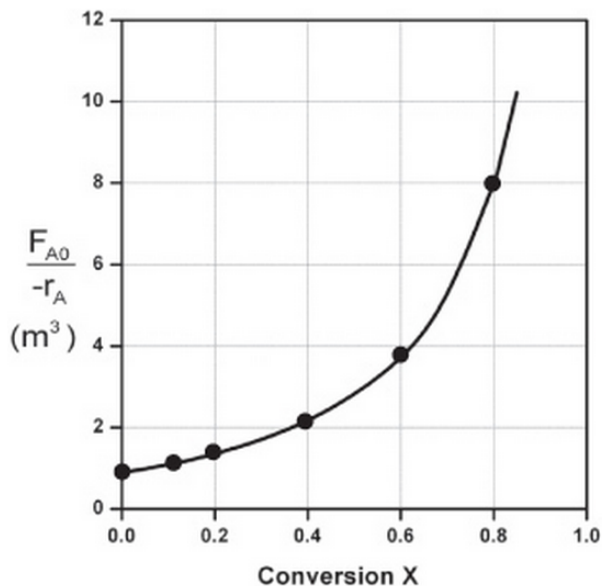
# Example: data collected

**Table 2-2. Processed Data**

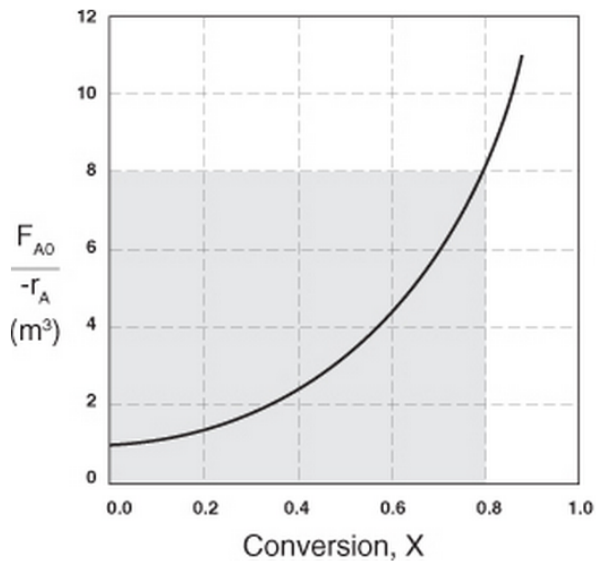
$X$	0.0	0.1	0.2	0.4	0.6	0.7	0.8
$-r_A \left( \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_A) \left( \frac{\text{m}^3 \cdot \text{s}}{\text{mol}} \right)$	2.22	2.70	3.33	5.13	8.85	12.7	20
$(F_{A0}/-r_A)(\text{m}^3)$	0.89	1.08	1.33	2.05	3.54	5.06	8.0

- ▶  $F_{A0} = 0.4 \text{ mol} \cdot \text{s}^{-1}$
- ▶ Isothermal and constant pressure; gas-phase
- ▶ We have **no idea what the reaction order is**

## Example: plotted

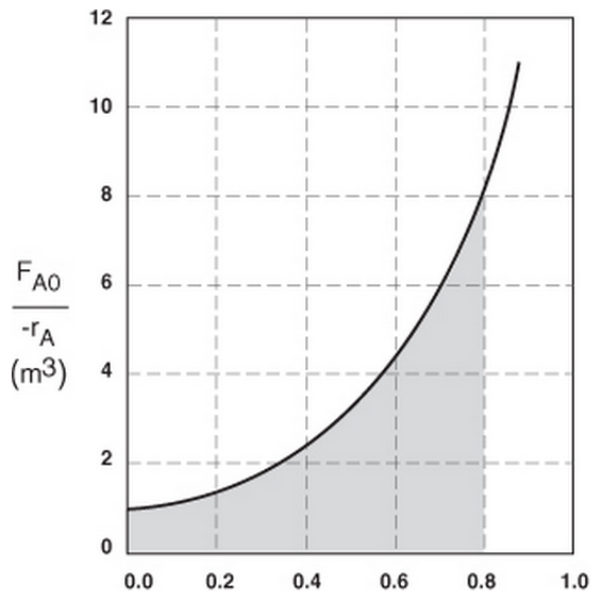


# CSTR solution



$$V_{\text{CSTR}} = 6.4 \text{ m}^3$$

# PFR solution



$$V_{PFR} = 2.165 \text{ m}^3$$



# Simpson's rules

- ▶ Got 3 equally-spaced points; with spacing =  $h$ ?

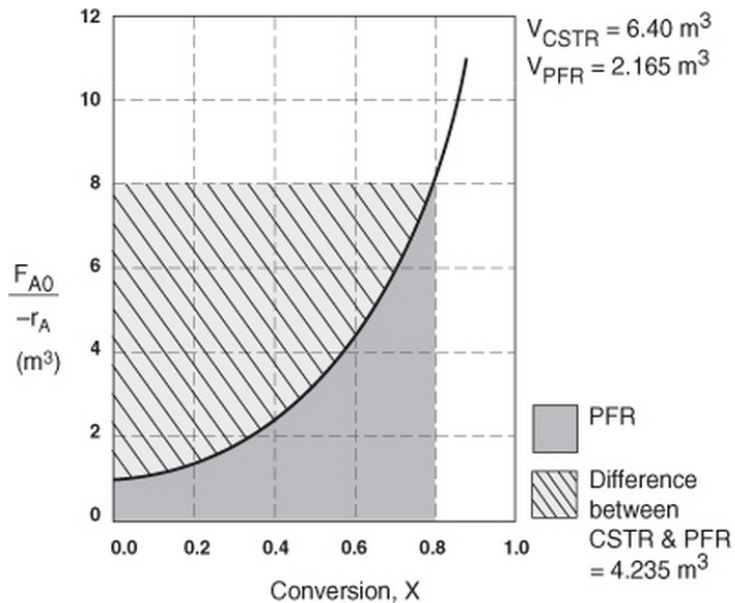
$$\int_{x_0}^{x_2} f(x) dx \approx \frac{h}{3} \left[ f(x_0) + 4f(x_1) + f(x_2) \right]$$

- ▶ Got 4 equally-spaced points; with spacing =  $h$ ?

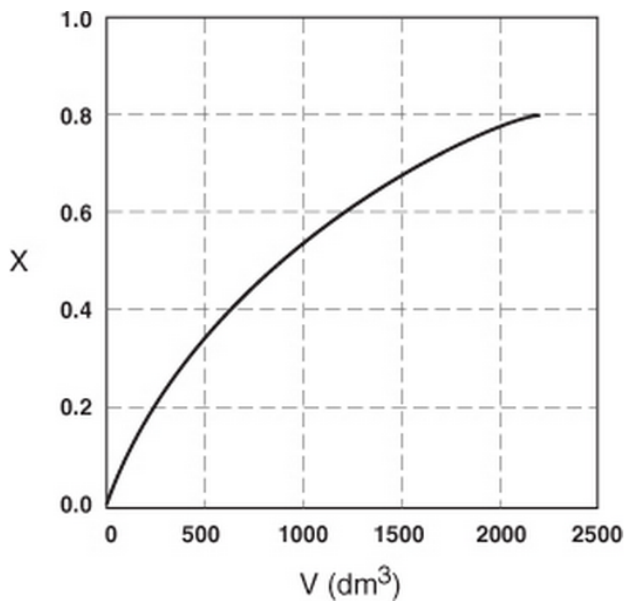
$$\int_{x_0}^{x_3} f(x) dx \approx \frac{3h}{8} \left[ f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right]$$

- ▶ See Appendix A for other formulas (more general)

# CSTR vs PFR



## Profiles along the reactor: $X$



## Profiles along the reactor: $r_A$

