# Introduction to Reactor Design ChE 3K4



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# 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

#### $aA + bB \longrightarrow cD + dD$

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 
    ightarrow 1 as  $t 
    ightarrow \infty$
  - For reversible reaction,  $X \to X_e$  (equilibrium conversion) as  $t \to \infty$
- 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

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

$$\begin{pmatrix} \text{moles } A \text{ at} \\ \text{time } t \end{pmatrix} = \begin{pmatrix} \text{initial} \\ \text{moles } A \end{pmatrix} - \begin{pmatrix} \text{moles } A \\ \text{consumed} \end{pmatrix}$$
$$N_A = N_{A0} - N_{A0} \cdot X$$
$$N_A = N_{A0}(1 - X)$$

## 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

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# Flow systems: CSTRs, PFRs and PBRs

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

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

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

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

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

Draw a picture here  $\rightarrow$ 

# 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<sub>A</sub>*: 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



Follows a similar derivation:

$$F_{A0}rac{dX}{dW}=-r_A'$$

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:

$$egin{aligned} \mathcal{F}_A &= \mathcal{F}_{A0}(1-X) \ \mathcal{C}_A &= rac{\mathcal{F}_A}{q} = rac{\mathcal{F}_{A0}(1-X)}{q} \end{aligned}$$

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

$$egin{aligned} \mathcal{C}_{\mathcal{A}} &= rac{\mathcal{F}_{\mathcal{A}0}}{q_0}(1-X) \ \mathcal{C}_{\mathcal{A}} &= \mathcal{C}_{\mathcal{A}0}(1-X) \end{aligned}$$

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
$-r_{\rm A}\left(\frac{\rm mol}{\rm m^3\cdot s}\right)$	0.45	0.37	0.30	0.195	0.113	0.079	0.05
$(1/-r_{\rm A})\left(\frac{{\rm m}^3\cdot {\rm s}}{{\rm mol}}\right)$	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

•  $F_{A0} = 0.4 \text{ mol.s}^{-1}$ 

- Isothermal and constant pressure; gas-phase
- We have no idea what the reaction order is

# Example: plotted



# Example: plotted (with best-fit line added)



# CSTR solution



## PFR solution



## 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: $r_A$



## Profiles along the reactor: X



How was this found?

### Reactors in series: multiple CSTRs South Africa, the Ergo tailings plant



### Flotation cells: Bolivia

#### See flotation cells in series on flickr.com

## Reactors in series: multiple CSTRs



# CSTR solution



### Rule for conversions in series

$$X_n = \frac{\text{total moles of A reacted leaving reactor } n}{\text{moles A fed to first reactor}}$$

e.g. for 2 reactors in series

$$egin{aligned} V_2 &= rac{F_{A1} - F_{A2}}{-r_{A2}} \ &= rac{F_{A0}(1-X_1) - F_{A0}(1-X_2)}{-r_{A2}} \ &= rac{F_{A0}(X_2 - X_1)}{-r_{A2}} \end{aligned}$$



### Reactors in series: multiple CSTRs

 Consider N CSTRs in series
 We observe that system approximates performance of a PFR of volume

$$V_{\mathsf{PFR}} \approx V_1 + V_2 + \cdots + V_N$$

Approximation improves as N increases.

### Homework exercise

- Example on page 56 (F2011)
- ► Example on page 62 (F2006)

#### 3 reactors in series



#### 3 reactors in series



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## Some further definitions

#### Space time, or residence time:

$$au = rac{V}{q_0}$$

time necessary to process one reactor volume of fluid based on entrance conditions