

# CHE 349: Kinetics and Reactor Design

## Lecture 1

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# Administrative Matters

- Get to Know Each Other
- Course Web Page:
  - <http://web.njit.edu/~jingwu/che349/index.html>
- Course Syllabus and Calendar
- Discuss Course Requirements and Grading Policy

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# Materials and Expectations

- Text Book
  - Elements of Chemical Reaction Engineering by H. Scott Fogler
- The CD-ROM
- Polymath and MatLab
- Class Room Participation: Ask Questions and Answer Questions
- Finish Homework and Required Reading in Time

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# Assignments Week 1

- Required Reading
  - Lecture 1: Sec. 1.1; Sec. 1.5; Sec. 3.1; Appendix A
  - Lecture 2: Sec. 1.2-1.4; Sec. 2.1 – Sec. 2.5, P129-P137.
- Homework I
  - Lecture 1: PI-3, PI-5, PI-II
  - Lecture 1: Familiar yourself with Polymath or MatLab.
  - Lecture 2: P2-3, P2-12

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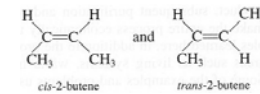
## Why Study Reaction Engineering (R. E.)

- It is the knowledge that distinguishes chemical engineers from others.
- It is the heart of producing all chemicals.
- It is the necessary knowledge for safe and efficient operation of a chemical plant.
- Its principle applies to
  - Petroleum Industry and Chemical Industry
  - Living Systems
  - Waste Treatment
  - Semiconductor Industry

## Basic Concepts in R. E. (I)

- Chemical Species Involved in a Reaction System: (Sec. 1.1, Pages 2-3)

The identity of a chemical species is determined by the kind, number and configuration of that species' atoms.



## Basic Concepts in R. E. (II)

- Chemical Reaction: (Sec. 1.1, Pages 2-3)  
A detectable number of molecules of one or more species have lost their identity and assumed a new identity



- Classification of Chemical Reactions: (Sec. 3.1 Page 68)
  - Homogeneous vs. Heterogeneous Reactions  
(Gas/Liquid Phase Reactions; Gas-Solid Phase Catalytic Reactions)
  - Reversible and Irreversible Reactions

## A Simplified Roadmap of R. E.

### Chemical Species and Chemical Reactions

#### Reaction Rate & Mechanism

- The path that a reaction follows.
- The rate of chemical reaction.

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

Typically expressed in differential forms and concerns chemical reaction at a point of a reactor

#### Reaction Engineering

- The principles for sizing of chemical reactors.
- Effects of heat of reaction.
- Diffusion and other transport effects on heterogeneous reactions.
- Nonideal reactors.

Typically expressed in integral forms and concerns integral/cumulative effects of chemical reactions in a reactor

## Stoichiometry and Reaction Rate

- Stoichiometry and Limiting Species



- Reaction Rate

- For homogeneous reactions, it is defined as the number of molecules disappeared or produced per unit time per unit volume. [mol/s dm<sup>3</sup>]
- Its definition depends on a reactor flow condition. For a constant volume batch reactor:

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

- $\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}$  Select one species, usually the limiting species, as the basis of calculation.

## Reaction Rate Constant & Rate Laws

- How the rate of a reaction is determined ?



- Temperature
- Concentrations of Reacting Species

$$-r_A = k_A(T) f_n(C_A, C_B, \dots)$$

- Rate Law:  $f_n(C_A, C_B, \dots)$
- Specific Reaction Rate (Constant):  $k_A(T)$

$$k_A(T) = A e^{-E/RT}$$

Under a specific temperature,  $k_A$  can be taken as a constant

## Reaction Order

- The Reaction Order

$$-r_A = k_A C_A^\alpha C_B^\beta$$

- The reaction order w. r. t. A is  $\alpha$ .
- The reaction order w. r. t. B is  $\beta$ .
- The overall reaction order is  $\alpha + \beta$ .
- Zero-order Reaction  $-r_A = k_A$
- First-order Reaction  $-r_A = k_A C_A$
- Second-order Reaction  $-r_A = k_A C_A^2$
- Third-order Reaction  $-r_A = k_A C_A^3$

## Exercise

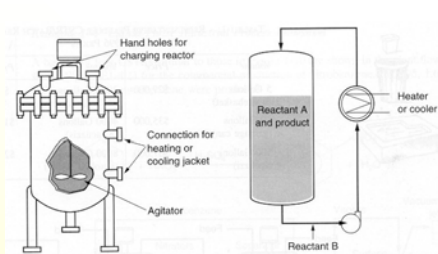
- Given:

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

Calculate concentration profile w. r. t. time if the reaction is:

- Zero-order Reaction  $-r_A = k_A$
- First-order Reaction  $-r_A = k_A C_A$
- Second-order Reaction  $-r_A = k_A C_A^2$
- Third-order Reaction  $-r_A = k_A C_A^3$

## Batch Reactors



Represent Batch Reactor by:



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## Why Batch Reactors



It is used for

- Small Scale Operations
- Intermediate or One Shot Production
- Pharmaceutical/Fermentation
- Gas/Liquid/Liquid-Solid Phase Reaction

Advantage:

- High Conversion
- Operational Flexibility

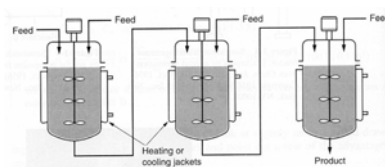
Disadvantage:

- High Labor Cost
- Product quality may vary.
- Difficult to Achieve Large Scale Production

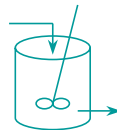
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## Continuous-Stirred Tank Reactor (CSTR)



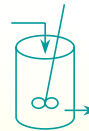
Represent CSTR by:



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## Why CSTR



It is used for

- Processes requiring agitation
- Liquid/Gas-Liquid/Solid-Liquid Reactions

Advantage:

- Continuous Operation
- Good Temperature Control
- Low Cost

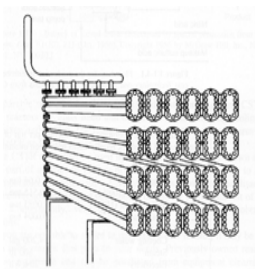
Disadvantage:

- Low Conversion

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## Plug Flow Reactors (PFR)



Represent PFR by:



## Why PFR



It is used for

- Gas-Phase Reactions
- Large Scale, Fast Reactions

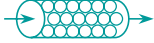
Advantage:

- Continuous Operations
- Relatively Easy to Maintain
- High Conversion
- Low Operating Cost

Disadvantage:

- Difficult to Control Temperature

## Other Reactors

- Semibatch Reactors
  - Either one reactant is charged and the other is fed continuously or one of the products can be removed continuously.
- Tubular Fixed Bed Reactor 
  - Tubular reactors that is packed with solid catalyst particles
- Fluidized Bed Reactor
  - A heterogeneous reaction takes place when catalyst particles are fluidized.

## Industrial Reactors (I)



## Industrial Reactors (II)



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