ChBE 4300 Kinetics and Reactor Design (required course)

Credit: 3-0-3

Prerequisite(s): Thermodynamics II (ChBE 3110), minimum grade of “C” and
Transport Phenomena I (ChBE 3200), minimum grade “C”. Transport Phenomena II (ChBE 3210) is a co-requisite.

Catalog Description

Reacting systems are analyzed in terms of reaction mechanisms, kinetics, and reactor design. Both homogeneous and heterogeneous reactions are considered.

Text

Chemical Reaction Engineering, Levenspiel, O., John Wiley, 3rd edition, 1999.

Objectives

This course introduces two basic concepts: (i) reaction mechanisms and kinetic rate expressions for homogeneous and heterogeneous reacting systems, including enzyme-catalyzed reactions and cell growth kinetics, and (ii) reactor design for the homogeneous reaction systems. The design principles for ideal homogeneous reactors are introduced, followed by the concept of RTD (residence time distribution) to diagnose and account for the non-idealities in flow patterns. For heterogeneous reactions, the role of transport (diffusion) effects, Thiele modulus, and catalyst effectiveness factor are introduced.

Learning Outcomes

By the end of this course, a student should be able to:

1. Analyze reaction mechanisms for homogeneous & heterogeneous reactions and develop kinetic rate expressions for the reactions. (Student Outcomes: a)
2. Develop microscopic and macroscopic mass and energy balances for various reactor types and identify the initial and boundary conditions (Student Outcomes: a, k)
3. Discern reaction kinetics by analyzing data from a variety of reactor types (Student Outcomes: a, b, e, k)
4. Design ideal isothermal reactors (Student Outcomes: c, e, k)
5. Design non-isothermal reactors by accounting for the heat effects (endothermic or exothermic reactions) as well as non-adiabatic reactor configurations (Student Outcomes: a, c, e, k)
6. Analyze RTD (residence time distribution) data to identify non-idealities in reactor configurations and utilize this information to predict reactor

performance (Student Outcomes: a, b, c. e, k)

7. Analyze for the role of transport effects in isothermal heterogeneous reactions. (Student Outcomes: a, b, c, e, k)

Topical Outline

1. Reaction Thermodynamics
    a. Heat of reaction effects
    b. Reaction free energy and equilibrium constant
    c. Effect of pressure and temperature on equilibrium conversion
2. Theories and Mechanisms of Homogeneous Reactions
    a. Bimolecular collision theory and Transition state theory
    b. Reaction intermediates and Bodenstein steady-state approximation
    c. Chain and non-chain reactions
    d. Kinetic rate expressions derived from reaction mechanisms
    e. Michaelis-Menten kinetics
3. Definitions of Rate and Design Equations in Different Reactor Types
    a. Mass balances around ideal homogeneous reactors
    b. Fractional conversion as a design variable in single reactions
    c. Integration of kinetics into the reactor design equation
    d. Graphical interpretation of reactor design equations
4. Multiple Reactions in Homogeneous Reactors
    a. Series vs. parallel reactions
    b. Yield and selectivity in multiple reactions
    c. Reactor design considerations
5. Non-isothermal Homogeneous Reactor Design
    a. Energy balances around non-adiabatic reactors
    b. Numerical vs. graphical approach to reactor design
    c. Multiple reactions in a non-isothermal reactor
6. Non-idealities in Homogeneous Reactors
    a. Residence time distribution (RTD)
    b. Segregated flow model
    c. Axial dispersion model
    d. CSTR's in series model
7. Heterogeneous Reactions
    a. Reaction mechanisms
    b. Langmuir-Hinshelwood kinetics
    c. Catalyst structure and transport
    d. Single pore diffusion model
    e. Thiele modulus and catalyst effectiveness factor

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