

# CHEMICAL REACTION ENGINEERING II

## ENCH 354

**Lecture** : 3  
**Tutorial** : 1  
**Practical** : 3/2

**Year** : III  
**Part** : II

### Course Objectives:

The objective of this course is to familiarize students with fundamentals of reaction mechanism, non-elementary rate laws, energy balance in reactors, reaction with catalysts, bioreactions, diffusion effects on heterogeneous reactions and residence time distribution in chemical reactors.

- 1 Reaction Mechanisms, Pathways, Bioreactions, and Bioreactor (10 hours)**
  - 1.1 Active intermediates and nonelementary rate laws
  - 1.2 Enzymatic reaction fundamentals
  - 1.3 Inhibition of enzyme reactions
  - 1.4 Bioreactors and biosynthesis
  
- 2 Catalysis and Catalytic reactors (8 hours)**
  - 2.1 Catalysts
  - 2.2 Steps in a catalytic reaction
  - 2.3 Synthesizing a rate law, mechanism, and rate-limiting step
  - 2.4 Heterogeneous data analysis for reactor design
  - 2.5 Catalyst deactivation
  
- 3 Steady State Non Isothermal Reactor Design (9 hours)**
  - 3.1 Steady state energy balance
  - 3.2 Adiabatic operation and equilibrium conversion
  - 3.3 Tubular reactors with heat exchange
  
- 4 Unsteady State Non Isothermal Reactor Design (4 hours)**
  - 4.1 Unsteady state energy balance
  - 4.2 Energy balance on batch reactors
  
- 5 Diffusion and Reaction (4 hours)**
  - 5.1 Diffusion and reaction in catalyst pellets
  - 5.2 External resistance to mass transfer
  - 5.3 Overall effectiveness factor

## 6 Residence Time Distribution

(10 hours)

- 6.1 Residence time distribution (RTD) function
- 6.2 Measurement and characteristics of the RTD
- 6.3 RTD in ideal reactors (Batch, CSTR, PFR)
- 6.4 Reactor modeling with RTD
- 6.5 Zero parameter models

### Tutorial

(15 hours)

1. Mathematical derivation of complex rate equations from a series of proposed reaction steps using pseudo steady state hypothesis
2. Calculation of reactor size, temperature, and conversion by balancing mass and energy
3. Numerical on deriving Langmuir-Hinshelwood (LHHW) rate laws, Thiele Modulus and effectiveness factor for a porous catalyst pellet
4. Michaelis-Menten equation and Lineweaver-Burk plot
5. Computational tools to solve differential unsteady reaction equations
6. RTD and Zero parameter models to determine conversion in a real reactor

### Practical

(22.5 hours)

1. Determination of the reaction rate constant in a stirred batch reactor
2. Evaluation of effect of reactant concentration on the reaction rate by using batch reactor
3. Evaluation of reaction rate constant in a continuous stirred tank reactor
4. Determination of the effect of inadequate mixing on the reaction rate using stirred tank reactor
5. Determination of the rate constant using tubular reactor
6. Demonstration of the temperature dependence of the reaction and the rate constant using tubular reactor
7. Characterization of pressure drops through fixed and fluidized bed

### Final Exam

The questions will cover all the chapters in the syllabus. The evaluation scheme will be as indicated in the table below:

| Chapter      | Hours     | Mark distribution* |
|--------------|-----------|--------------------|
| 1            | 10        | 13                 |
| 2            | 8         | 12                 |
| 3            | 9         | 12                 |
| 4            | 4         | 5                  |
| 5            | 4         | 5                  |
| 6            | 10        | 13                 |
| <b>Total</b> | <b>45</b> | <b>60</b>          |

\* There may be minor deviation in marks distribution.

## References

1. Fogler, H. S. (2016). Elements of chemical reaction engineering. Prentice Hall.
2. Levenspiel, O. (1999). Chemical reaction engineering. John Wiley & Sons. (Latest Edition)