

## CHE-976 Advanced Chemical Kinetics & Its Applications

**Credit Hours:** 3

**Pre-requisites:** Nil

### **Course Objectives:**

- Imparting basic to advance knowledge of kinetics to the students.
- Examples from the industry for incorporation of principle of Kinetics learned during the course.
- Up gradation of existing processes through research work based on the knowledge learned.

### **Course Contents:**

#### **Introduction to Chemical Kinetics:**

Rate of Reaction, Rate constant, Order and Molecularity, Various order of reaction, The effect of temperature on reaction rates.

#### **Kinetics and Thermodynamics:**

Thermodynamics and chemical reactions.

#### **Unimolecular Reactions:**

Lindemann theory, Hinshelwood theory, RRKM Theory.

#### **Kinetics aspects of Mass Spectrometry:**

Quasi Equilibrium theory, Mass Spectrometry Basics, Kinetic studies employing Mass spectrometry.

#### **Thermal Analytical Techniques and Kinetic studies:**

Basic principles of thermal analytical techniques, Arrhenius equation, Determination of Arrhenius parameters.

#### **Kinetics of Polymerization:**

Types of polymerizations, Kinetics of free radical polymerization, Co-polymerization

#### **Investigation of Mechanism by Kinetic Methods:**

The reaction of acetone with Iodine, Nitration of aromatics hydrocarbons, The thermal decomposition of Dinitrogen Pentoxide.

#### **The Kinetic isotope effect:**

The kinetic isotope effect, The reverse kinetic isotope effect.

#### **Fast Reactions:**

Introduction, Flow techniques, Relaxation method, Shock tubes, ESR spectroscopic techniques, NMR spectroscopic techniques

Analysis of Experimental Results

### **Course Outcomes:**

- Understanding the heart of Chemistry and Chemical Engineering principles.
- Determination of Arrhenius parameters.
- Design of chemical reactors.

### **Recommended Reading (including Textbooks and Reference books)**

- Elementary reaction kinetics, Latham, Joseph Lionel
- Chemical Kinetics and reaction dynamics, Santosh K. Upadhyay
- Modern methods in Kinetics, C.H. Bamford and C.F.H Tipper-Editors
- Chemical Engineering Kinetics, Smith, J.M.
- Introduction to chemical engineering kinetics and reactor design, 2<sup>nd</sup> edition, Wiley.