Title : Chemical Kinetics and Reaction Dynamics
Code : CSE-871
Credit Hours: 3-0

Description: This course is designed to introduce the students with reaction mechanisms, identify the reaction intermediates, determine the molecularity of each elementary reaction, and to determine transition states and activation energy using computational tools.

Objectives:

Main Objectives of the program under which course will be designed are;

1. Introducing definition Chemical Kinetics and Dynamics and understanding of Rates of Chemical processes.
2. Use concentration versus time data to calculate an average rate of reaction over a period of time
3. Construction of mathematical models for simulation of transition state and calculation of activation energy.

Outcomes: After successful completion of course, students will be able to

- Analyse a scientific study of the kinetics of a chemical reaction.
- Apply and identify basic concepts related with chemical engineering.
- Apply the concepts of heterogeneous catalytic chemical kinetics.
- Apply the concepts of homogenous chemical kinetics.
- Develop independent learning strategies. Develop scientific thinking.

Course Contents:

1. Basic Concepts of Kinetics
2. Complex Reactions
3. Reactions in Solution
4. Potential Energy Surfaces
5. Catalysis
6. Dynamics of Bimolecular Collisions
7. Transition State Theory

Contents with proposed contact hours

Week	Topics
1	Definition of Rate of a Chemical Order and Molecularity of a Reaction
2	Integrated Reaction Rate Laws , Integrated Zero order (Thermal decomposition of HI on Au-Surface-using computational tool) 1^{st} order reactions (Isomerization of CH_3NC to CH_3CN-using computational tool)
3	Integrated 2^{nd} order reactions (Recombination of CH_3 free radicals) Integrated 3^{nd} order reactions,

4	Determination of Reaction Order:, Different methods to determine order of Reaction. half life method
5	Temperature dependence of Rate Constants: The Arrhenius Equation , Constant Coefficients, Undetermined Coefficients, Calculation of reactant, TS and product energies, rate constants *k* and activation energy (E_a)-using computational method
6	Complex Reactions, Reversible Reactions
7	Consecutive Reaction, Examples of a Complex Reaction Mechanism
8	Reactions in Solution, General Properties of Reactions in Solution,
9	**Mid Term**
10	Theory of Reaction Rates Diffusion limited Rate Constant, Effect of ionic strength on Reaction between ions
11	Potential Energy Surfaces, Long Range Potentials, Molecular Bonding Potentials
12	Intermolecular Potentials , *Ab-initio* Calculations of Potential Energy Surfaces,
13	Analytical Potential Energy Functions (Mapping potential energy surface to identify electrophilic and nucleophilic region.) (Calculation of potential energy contours)
14	Catalysis and Dynamics, Homogenous catalysis, Heterogenous catalysis and Gas-Surface Reactions Enzyme-Catalyzed
15	Dynamics of Bimolecular Collisions Simple Collision Models Two Body classical Scattering Complex scattering Processes
16	Transition State Theory Motion on the Potential Surfaces Basic Postulates and derivation of Transition State Theory Transition state optimization and frequency calculations (ADF hands on)
17	Thermodynamic Formulation of Transition State Theory . Applications of Transition State Theory
18	**ESE**

Text Books/Reference Material:

1. Paul L. Houston (2006). *"Chemical Kinetics and Reaction Dynamics."* Mc Graw Hill Inc., New York.
2. Richard I. Masel (2002), *"Chemical Kinetics & Catalysis"* 1st Edition
3. Jaffrey I. Steinfeld (1999). "*Chemical Kinetics and Dynamics."* Prentice Hall Inc., USA.

4. S.R. Login (1996). *"Fundamental of Chemical Kinetics."*Addison Wesley
5. Upadhyay, Santosh K (2007). *"Chemical Kinetics and Reaction Dynamics".* Anamaya Publishers.
6. **Nature of Assessments:** Homework/

Assignments:	10%
Quizzes:	10%
MSE:	30%
Final Exam:	50%