Programme: M. Sc. Part-II (Chemistry)
Course Code: PCO-504 Title of the Course: Chemical kinetics and reaction dynamics
Number of Credits: 03
Effective from AY: 2019-20

Prerequisites for the course:	Students should have studied the course PCC- 401, PCO- 401 in Semester I/II, so as to have basic knowledge of reaction kinetics.	No. of lectures/hours
Course Objectives:	1. To introduce concepts of reaction kinetics and dynamics 2. To provide fundamental knowledge of theories that govern chemical reactions 3. To introduce newer classes of reaction types and their kinetics 4. To introduce latest developments in the advance instrumental techniques and methods for monitoring reaction kinetics and dynamics.	
Course Outcomes:	1. Students should be in a position to understand the concept of reaction kinetics and its significance. 2. Student will be able to differentiate between different reaction types, their kinetic analysis and its significance 3. Students should be able to apply these kinetic concepts to perform laboratory experiments in reaction kinetics. 3. Students should be in a position to apply these concepts of real life applications such as combustion engines, photochemical systems and atmospheric chemistry research.	
Content:	1.0 Theories of reaction rates 1.1 Generalized kinetic theory and extended collision theory. Concept of collisional number, collisional frequency factor, collisional and reactive cross section, steric factor, microscopic rate constant. Assumptions and limitations of collision theory 1.2 Conventional transition state theory, equilibrium hypothesis and derivation of reaction rates. Thermodynamic formulation of transition state theory. Arrhenius temperature dependent and independent activation energy and its significance. Assumptions and limitations of transition state theory. Introduction to extended transition state theory and microscopic reversibility. 1.3 Lindemann-Hinshelwood theory of thermal unimolecular reactions. Statistical energy dependent rate constant. Introduction to RRK and RRKM Theory and its applications. 2.0 Elementary reactions in solutions 2.1 Collisional kinetics in solution, effect of solvent polarity solvent cohesion energy, influence of ionic strength and ion-dipole and dipole-dipole reactions on reaction rates. Comparison of gas phase and solution reactions. 3.0 Homogeneous and surface reactions	8 hr 3 hr 8 hr

	3.1 Homogeneous kinetics, enzymatic reactions and Michaelis-Menten, Lineweaver-Burk and Eadie Analysis 3.2 Autocatalytic and inhibition reactions. Product induced competitive and non-competitive inhibition reactions. 3.3 Adsorptions: competitive, non-ideal and dissociative adsorptions 3.4 Mechanism of surface reactions, kinetic effects of surface heterogeneity and interactions. 3.5 Eley-Rideal, Langmuir Hinshelwood and Mars van Krevelen kinetic models of surface reactions	
	4.0 Composite reactions 4.1 Types of composite mechanisms, rate equation for composite mechanisms, simultaneous and consecutive reactions 4.2 Decomposition reactions of ozone and acetaldehyde 4.3 Gas phase combustion reactions, hydrogen – oxygen combustion, introduction to shock tube method and its use in combustion analysis. 4.4 Polymerization kinetics, stepwise and chain polymerization.	4 hr
	5.0 Fast Reactions 5.1 Photochemical fast reactions: primary photochemical processes, reactions of electronically excited species and photochemical equivalence. 5.2 Pulsed laser photolysis, multiphoton excitation processes and its use in monitoring fast reactions. 5.3 Radiation-chemical reactions: radiation chemical primary processes, kinetic measurements in radiolysis method. 5.4 Comparison of relaxation method and stopped flow technique.	5 hr
	6.0 Reversible, Irreversible and Oscillatory reactions. 6.1 Kinetics of reversible, irreversible reactions and graphical analysis 6.2 Voltera-Lotka hypothesis of oscillatory reactions. The significance of bi-stability in the Briggs-Rauscher Reaction and Belousov-Zhabotinskii reaction.	4 hr
	7 Reaction Dynamics 7.1 Reactive collisions, chemiluminescence and laser induced fluorescence. 7.2 Introduction to potential energy surfaces, internal coordinates and modes of vibration with suitable examples. 7.3 Introduction to molecular reaction dynamics, investigation of reaction dynamics with ultrafast lasers.	4 hr

Pedagogy:	Mainly lectures / tutorials. Seminars / assignments / presentations / self-study or a combination of some of these could also be used to some extent.	
Text Books / References	1. K. J. Laidler, *Chemical Kinetics, Pearson Education, 1987; (printed in India by Anand Sons,2004), 3rd edition*. 2. P.W. Atkins and J. De. Paulo, *Atkins' Physical Chemistry, Oxford University Press, 2007, 8th edition.* 3. J. I. Steinfeld, J. S. Francisco and W. L. Hase, *Chemical Kinetics and Dynamics, Prentice Hall, 1999, 2nd edition.* 4. D. K. Chakrabarty and B. Viswanathan, *Heterogeneous Catalysis, New Age International Publishers, 2008* 5. S. K. Scott, *Oscillations, waves and Chaos in chemical kinetics, Oxford Science Publications, 1994.* 6. Thomas S. Briggs, and Warren C. Rauscher, *An oscillating iodine clock, J. Chem. Educ., 1973, 50 (7), 496*	