

Semester	AUG 2022
Open to semester	5,7,11,13,21
Course code	<b>CH3154/CH6154</b>
Course title	<b>Chemical Equilibrium and Kinetics</b>
Credits	4 /4
Course Coordinator & participating faculty (if any)	Arnab Mukherjee
Nature of Course	Lectures
Pre-requisites	Thermodynamics (IDC) course
Objectives (goals, type of students for whom useful, outcome etc)	<p>This course is an advanced continuation of the one component-one phase thermodynamics introduced in the fourth semester. In this course, the application of thermodynamics to multicomponent (water/ethanol mixture or reaction mixture of multiple compounds), or multiphase (water/vapor mixture) systems is discussed with the help of Gibbs free energy or chemical potential. It is, however, emphasized the root of the changes that we observe in a multicomponent system (mixing or nonmixing of two liquids or formation of vapor pressure) is the underlying consequence of the entropy of the universe as a driving force.</p> <p>Therefore, this course will help us understand why a certain reaction will happen, how the volumes of two mixtures will change, and what kinds of phases will be produced in the mixture of liquids, gases, and solids. Moreover, what kinds of solution an electrolyte will make compared to that of a nonelectrolyte.</p> <p>After discussing the equilibrium states of ideal and nonideal mixtures, this course then will discuss the rate of change in these equilibrium states, known as chemical kinetics in which the rate laws of various chemical reactions, catalysis, etc. will be discussed. Finally, this course will discuss various reaction rate theories which are used even today to understand the rate of a chemical reaction.</p> <p>Thus the objective of this course is to give a consolidated picture of the equilibrium and kinetics of multicomponent mixtures in chemical systems.</p>
Course contents (details of	<ul style="list-style-type: none"> <li>• Review of thermodynamics of one component system:</li> </ul>

<p>topics /sections with no. of lectures for each)</p>	<p>Statement of three laws, the basic definition of entropy and its meaning, the fundamental equation of thermodynamics, Legendre transformation, free energies and their implications (2 hr)</p> <ul style="list-style-type: none"> <li>• Introduction to the multi-component system: Introduction to chemical potential and use it to define both chemical equilibria and phase equilibria, Gibbs-Duhem equation, the connection of chemical potential with partition function, problem-solving (3 hr)</li> <li>• Reaction equilibrium in ideal gas mixtures: Chemical potential in an ideal gas mixture, reaction equilibrium in a gas mixture, equilibrium constant and its dependence on temperature, van't Hoff equation, problem-solving (3 hr)</li> <li>• Phase equilibria in one component (multiphase) system: Phase rule, Clapeyron, and Clausius-Claperon equation, introduction to phase diagram, problem-solving (3 hr)</li> <li>• Ideal Nonelectrolytic Solutions: Partial molar thermodynamic quantities (volume, enthalpy, entropy, etc.), calculation of partial molar volume, thermodynamics of mixing, ideal solution and ideally dilute solution, calculation of vapor pressure, Raoult's law and Henry's law, problem-solving (5 hr)</li> <li>• Nonideal Solutions: Activity and activity coefficient from both convention I (deviation from ideal solution) and convention II (deviation from ideally dilute solution) excess function ( 6 hrs)</li> <li>• Nonideal electrolytic solution: Activity of electrolytes, Debye-Huckel theory, problem-solving (3 hrs)</li> <li>• Multicomponent Phase Equilibria: Colligative properties (vapor pressure lowering, freezing point depression, and osmosis), two-component phase diagram, two-component liquid-vapor, liquid-liquid (azeotropic composition), solid-liquid phase diagrams (eutectic and peritectic composition) and general discussion about other phase diagrams. (4 hr))</li> <li>• Chemical Equilibrium: Spontaneous chemical reaction, reaction equilibria in electrolyte and nonelectrolyte solution, in gas mixtures and in solids, temperature and pressure dependence of the equilibrium constant (3 hrs)</li> <li>• Equilibrium Electrochemistry: Half reactions and electrodes, varieties of cells, cell potentials, standard electrode potential, applications, and problem-solving (3 hrs)</li> <li>• Chemical Kinetics: Rate and order of a reaction,</li> </ul>
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	<p>experimental determination, mechanism of reactions (parallel, consecutive reactions), the temperature dependence of rate, unimolecular reaction, catalysis, enzyme catalysis (4 hrs)</p> <ul style="list-style-type: none"> <li>• Chemical Dynamics: Theories of reaction rate (collision theory, Eyring theory, and transition state theory) (3 hrs)</li> </ul>
Evaluation /assessment	<p>End-Sem Examination-40%</p> <p>Mid-Sem Examination-50%</p> <p>Others-10% will be from class quizzes%</p>
Suggested readings (with full list of authors, publisher, year, edn etc.)	<ol style="list-style-type: none"> <li>1. Physical Chemistry by Ira N. Levine, 6th edition, McGraw-Hill Higher Education Publication, (2008)</li> <li>2. Physical Chemistry by Peter Atkins and Julio de Paula, 9th Edition, W. H. Freeman and Company (2010)</li> <li>3. Physical Chemistry: A Molecular Approach by D. A. McQuarrie and J. D. Simon, University Science Books (1997).</li> </ol>