THERMODYNAMICS AND KINETICS

Course Type	Course Code	Name of the Course	L	T	P	Credits
DC	FMC205	**Thermodynamics and Kinetics**	3	0	0	9

Course Objective
Basic understanding of the laws of thermodynamics and equilibrium in chemical/metallurgical systems and chemical reaction kinetics.
Learning Outcomes
• Laws of thermodynamics and its applications, equilibrium in chemical reactions, phase equilibria in one and two component systems. • Rate law in chemical reaction kinetics, definition, and basic design of ideal and non-ideal reactors.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1.	Importance of thermodynamics; basic definitions: universe, system, surroundings, boundary, homogeneous and heterogeneous systems, intensive and extensive properties, state and path functions, classification of processes, zeroth law of thermodynamics; equations of state; mixture of ideal gases; real gases.	2	Introduction to thermodynamics and associated terminology.
2.	Work and heat; state and path functions; reversible and irreversible processes; first law of thermodynamics; internal energy; enthalpy; isothermal and adiabatic expansion; JouleThomson expansion; examples of some thermodynamic cycles	4	Concepts and applications related to the first law of thermodynamics.
3.	Second law of thermodynamics; heat engines; Carnot cycle; concept of entropy; criterion for equilibrium; entropy and disorder; Gibbs free energy; Maxwell's relations; GibbsHelmholtz equation	7	Concepts and applications related to the second law of thermodynamics and criteria for equilibrium.
4.	Heat of formation; heat of reaction; heat capacity; Hess's law; third law of thermodynamics; calorimetry	4	Calculation and measurement of enthalpy changes in endothermic and exothermic reactions.
5.	Multicomponent systems; partial molar quantities; chemical potential; Gibbs-Duhem equation; homogeneous and heterogeneous chemical equilibrium	4	Concepts related to equilibrium in multicomponent systems
6.	One-component phase equilibria: phase diagram; Gibbs phase rule; Clayperon equation; critical point and supercritical fluids; Clausius-Clayperon equation	4	Understand phase transition and phase co-existence in a one-component system
7.	Two-component phase equilibria: Ellingham diagram; Raoult's law; Henry's law; concept of activity, Gibbs-Duhem equation, regular solution, phase diagram, Lever's rule; Sievert's law	7	Understand phase equilibrium in gas-solid and gas-liquid systems
8.	Thermodynamics versus kinetics; reaction mechanism in homogeneous and heterogeneous systems; rate controlling step; rate equation; experimental determination of rate equation parameters; batch and continuous reactors; stirred tank reactors; plug flow reactors; reactor conversion and sizing; residence time distribution.	10	Fundamentals of chemical reaction kinetics and its application in ideal/non-ideal reactors
	Total	42	

Text Books:

1. Lecture Notes | Thermodynamics & Kinetics | Chemistry | MIT OpenCourseWare (https://ocw.mit.edu/courses/chemistry/5-60- thermodynamicskinetics-spring-2008/lecture-notes/)

Reference Books:

1. Introduction to the Thermodynamics of Materials, D. R. Gaskell & D. E. Laughlin, CRC Press
2. Elements of chemical reaction engineering, H. Scott Fogler, Prentice Hall.