

GUJARAT TECHNOLOGICAL UNIVERSITY

Thermodynamics of Elastomers & Polymers

SUBJECT NAME: Rubber Technology

SUBJECT CODE: 2132603

B.E. 3RD SEMESTER

Type of course: Core-III (B. E. Rubber Technology)

Prerequisite:

Rationale:

Teaching and Examination Scheme:

Teaching Scheme			Credits C	Examination Marks						Total Marks
L	T	P		Theory Marks			Practical Marks			
				ESE (E)	PA (M)		PA (V)		PA (I)	
		PA	ALA		ESE	OEP				
4	2	0	6	70	20	10	30	0	20	150

L- Lectures; T- Tutorial/Teacher Guided Student Activity; P- Practical; C- Credit; ESE- End Semester Examination; PA- Progressive Assessment; OEP-Open Ended problem; AL-Active learning;

Content:

Sr. No.	Content	Total Hrs	% Weightage
1	Basic Concepts of Thermodynamics: Terminology of thermodynamics, Zeroth law, first law of thermodynamics, enthalpy, reversible isotherm, expansion of an ideal gas, Thermo chemical definition, Hess's law of constant heat summation, heat capacity, relation between C_v & C_p , adiabatic expansion of an ideal gas, Kirchoff's equation, flame & explosion temperature, Joule-Thomson effect, Carnot's theorem Second Law of thermodynamics & Entropy, Second law of thermodynamics, Concept of entropy, entropy change in reversible & irreversible process, entropy of phase transition, entropy change for an ideal gases, entropy change during mixing of ideal gases, free energy & its change of an ideal gas in isothermal change, Gibbs-Helmholtz equation, Maxwell's thermodynamic relations, Clapeyron-clausius equation, Van't hoff isotherm.	10	15
2	Fundamental Principles: Balance Equations, Basic thermodynamics for Rubber Elasticity & Strain induced Crystallization. Basics of Devolatilization, Devolatilization of Particulate polymer, Devolatilization of Polymer Melts, Pipe Flow of Newtonian Fluid.	08	05
3	Heat of Polymerization: Heat of Polymerization (ΔH_p), Factors affecting ΔH_p . Variations in Heat of Polymerization. Estimation of Heat of Polymerization.	06	10
4	Ceiling Temperature: Concept of Ceiling Temperature, Spontaneity, Conditions for Polymerization Reaction.	04	05
5	Energy Balances: Introduction, energy & thermo chemistry, Energy balances, Heat capacity,	06	10

	Latent Heats, Absolute Enthalpy, Adiabatic reactions, dissolution of solids, Absorption, evaporation.		
6	Polymer Chain Flexibility: Internal rotation in Molecules, Rotation barrier, configuration & conformation of molecules & Macromolecules, internal rotation in macromolecules, dimensions of macromolecular coils, Thermodynamic Flexibility of a Chain, Kinetic Flexibility of a chain & factors determining it, Practical Importance of Chain flexibility in elastomers.	06	10
7	Theory of Polymer Solutions: Basic concepts solutions, Polymer solutions. Effect of Crosslinking on Solubility, Solubility Parameter, Flory-Huggins theory: Entropy of mixing on formation of an Thermal solution, change in Gibbs Free Energy on Dissolution of Polymers, Phase equilibrium in polymer solutions, theory of dilute polymer solution, statistical theory of swelling of network polymers, Merits of polymer solutions, Prigogine's Theory: pure liquids with chain molecules, law of principle of corresponding states, Thermodynamics of Mixtures of Liquids with Chain Molecules.	06	10
8	Thermodynamics of Polymer Solutions: Partial Molar (Specific) Functions, Methods of Calculating Partial Equations, Ideal & Nonideal Solutions, Thermodynamic Affinity of a solvent to a polymer or Thermodynamic Quality of a solvent, Vapor Pressure over Polymer solutions, Osmotic Pressure, Swelling Pressure, Second Virial Coefficient, Free Energy of Mixing of a polymer with a solvent, Thermodynamic Stability of Systems, Enthalpy or Heat of Mixing, Differential Heats of Solutions & Dilution, Entropy of Mixing, Change in Volume or Dissolution of Polymers, Internal energy of Mixing, Variation of Thermodynamic Affinity of a polymer to a solvent with temperature criteria of UCST & LCST, Thermodynamics of Dissolution of Polymers & their structure, Thermodynamics of Swelling of Cross linked Polymers.	08	10
9	Combustion: Introduction, Fuels, Calorific values of fuels, coal, liquid fuels, gaseous fuels, air requirement & flue gases, combustion calculations.	08	10
10	Thermodynamics Investigation of Polymer-Polymer Systems. Three- component Systems.	02	05
	Thermodynamics of Binary Polymer-Polymer Systems :- Enthalpy of Mixing of Two Polymers, Free Energy of Mixing of Polymers, Entropy of Mixing of Two Polymers, Phase Diagrams of Polymer-Polymer Systems.	04	05
	Thermodynamic Properties: Relationship between molecular weight and two fundamental thermodynamic properties (1) Thermal conductivity (2) Coefficient of Thermal Expansion., Thermodynamic forces favoring maximum potential crystallinity.	04	05

Reference Books:

- 1) Physical Chemistry of Polymers, by A. TAGER, MIR Publishers-Moscow
- 2) Engineering Chemistry by Jain & Jain
- 3) Polymer Extrusion by Chris Rauwendaal
- 4) Polymer Processing Principles and Design, by Donald G. Baird, Dimitris I. Collias
- 5) Polymer Structure, Properties and Applications by RUDOLPH D. DENIM
- 6) Thermodynamics of Polymerization', Hideo Sawada.

Course Outcome:

After learning the course the students should be able to:

- Understand the importance of reversible & irreversible process of energy.
- Define the heat of polymerisation and influencing factors.
- Apply the statistical theory of swelling of network polymers.
- Identify the merits & demerits of polymer solutions.
- The course will be helpful to design the models for elastomers based on fundamental of thermodynamic properties.
- Understand the different laws of thermodynamics.
- Learn about basic concept of thermodynamics for rubber elasticity.
- Analyze the conditions for polymerisation reaction.
- Compare Configuration & conformation of molecules & Macromolecules.
- Study the concept of solubility parameter.
- Learn the thermodynamics of mixture of liquids.
- Distinguish various terms like vapour pressure, osmotic pressure and swelling pressure.
- Know about the Dissolution of Polymers & their structure in term of thermodynamics.

List of Experiments:

Tutorials based on above topics.

List of Open Source Software/learning website:

- link.springer.com/article/10.1007%2Fs002890050457
- wolf.chemie.uni-mainz.de/.../thermodynamics_of_polymer_solutions.pdf
- fluid.wme.pwr.wroc.pl/.../combustion.../LIQUID_FUEL_COMBUSTION
- www.chem.ufl.edu/~itl/4411L_f96/rubber/rubber_sav.html
- www.boundless.com > ... > The Laws of Thermodynamics

Active learning Assignments (AL) : Preparation of power-point slides, which include videos, animations, pictures, graphics for better understanding theory and practical work – The faculty will allocate chapters/ parts of chapters to groups of students so that the entire syllabus to be covered. The Power-point slides should be put up on the web-site of the College/ Institute, along with the names of the students of the group, the name of the faculty, Department and College on the first slide. The best three works should submit to GTU