

GUJARAT TECHNOLOGICAL UNIVERSITY

CHEMICAL ENGINEERING (COMPUTER AIDED PROCESS DESIGN) (16)

PROPERTY PREDICTION FOR MIXTURES (PPM)

SUBJECT CODE: 2721604

SEMESTER: II

Type of course: (Major Elective-III) (M.E.CAPD)

Prerequisite: Energy & Mass Integration (EMI)

Rationale: Understand the Fundamental thermodynamic relations.

Teaching and Examination Scheme:

Teaching Scheme			Credits C	Examination Marks						Total Marks
L	T	P		Theory Marks		Practical Marks				
			ESE (E)	PA (M)	ESE (V)		PA (I)			
					ESE	OEP	PA	RP		
3	2#	0	4	70	30	30	0	10	10	150

Content:

Sr. No.	Topics	Teaching Hrs.	Module Weightage
1	Estimation and Computation of Thermodynamic and Transport Properties: Estimation of Properties - Density, Viscosity, Thermal conductivity, Enthalpy, K-value, Diffusivity, Surface Tension, Types of Estimations, estimation of pure component constants, Mixing rules.	6	10
2	Density: Densities of Gas using equations of state, estimation of liquid densities by HBT method, Rackett techniques, Bhirud method, densities of liquid mixtures, effect of temperature and pressure.	6	10
3	Fluid Phase Equilibrium Prosperities: Thermodynamics of VLE, fugacity and activity coefficients, binary VLE, multi-component VLE, solubility of gases in liquids, liquid-liquid equilibrium.	6	10
4	Heat Capacity and Enthalpy: Fundamental thermodynamic relations, departure functions, heat capacity of gases and liquids, enthalpy of vaporization, estimation of boiling point	6	10
5	Viscosity: Theory of gas transport properties, estimation of low-pressure viscosity for pure gas and mixture, effect of pressure, viscosity at high pressure, liquid viscosity, effect of temp and pressure on liquid viscosity, liquid mixture viscosity.	6	10
6	Thermal Conductivity: Theory of thermal conductivity, thermal conductivity of poly atomic Gases, effect of temperature and pressure, thermal conductivity of liquids, estimation of thermal conductivity for pure liquids and liquid mixtures	6	10
7	Diffusion Coefficient: Diffusion coefficient for binary Gas systems, effect of temperature and pressure, diffusion in multi-component gas, estimation of liquid diffusivity,	6	10

	effect of concentration and temperature, diffusion in multi-component liquid mixtures and in electrolytes.		
8	Surface Tension: Estimation of the surface tension for pure liquids, effect of temperature, surface tension of aqueous and non-aqueous solutions.	6	10
9	Selection of thermodynamic Model/Method: Selection of best proper property prediction method for available data, limitations and advantages of methods, data sources, computer database / programs for property estimation.	6	15

Reference Books:

1. The Properties of Gases & Liquids, Robert C Reid, John M Prausnitz and Bruce E. Poling by McGraw-Hill
2. Perry's Chemical Engineers' Handbook, Perry, R.H.; Green, D.W. by McGraw-Hill

Course Outcome:

After learning the course the students should be able to:

- Learn about the Types of Estimations, estimation of pure component constants.
- Understand the Fundamental thermodynamic relations.
- Learn about Thermodynamics of VLE, fugacity and activity coefficients.
- Study about the Estimation of low-pressure viscosity for pure gas and mixture,
- Learn the diffusion in multi-component liquid mixtures and in electrolytes.
- Know about the Estimation of the surface tension for pure liquids.
- Identify the Selection of best proper property prediction method for available data.
- Study about computer database / programs for property estimation..
- Understand the surface tension of aqueous and non-aqueous solutions.

Major Equipment:

Emissivity Measurement Apparatus, Kinematic Viscometer Bath, Flow Cup Viscometer etc.

List of Open Source Software/learning website:

- www.just.edu.jo/~yahussain/files/Thermodynamic%20Models.pdf
- support.olisystems.com/Documents/.../Shock1988GeochimCosmo2009.p
- etd.nd.edu/ETD-db/theses/available/etd.../JayaramanS082009D.pdf
- www.wag.caltech.edu/publications/sup/pdf/419.pdf

Review Presentation (RP): The concerned faculty member shall provide the list of peer reviewed Journals and Tier-I and Tier-II Conferences relating to the subject (or relating to the area of thesis for seminar) to the students in the beginning of the semester. The same list will be uploaded on GTU website during the first two weeks of the start of the semester. Every student or a group of students shall critically study 2 papers, integrate the details and make presentation in the last two weeks of the semester. The GTU marks entry portal will allow entry of marks only after uploading of the best 3 presentations. A unique id number will be generated only after uploading the presentations. Thereafter the entry of marks will be allowed. The best 3 presentations of each college will be uploaded on GTU website.