Department of Chemical Engineering

PhD Admission

Area of Research:

Chemical Engineering: Mass Transfer, Catalysis, Environmental Pollution Control, Bioreactors.

Polymer Science and Technology: Chemical sensor, Nanocomposites, Hydrogels, Biodegradable polymers, Polymeric Membranes, High performance composites, Biocomposite, Modified Polyolefins, Fire retardant filler, Lignin based printing inks/pigments, Material Process Modeling

Syllabus for Examination:

A. Polymer Science and Technology Back Ground:

Chemistry of high polymers: Monomers, functionality, degree of polymerizations, classification of polymers, glass transition, melting transition, criteria for rubberiness, Principle of polymerization, addition and condensation polymerization; their kinetics, chain transfer, inhibition and retardation, control of molecular weight, branching effects of addition/chain growth polymerization, metallocene polymers and other newer techniques of polymerization, copolymerization, monomer reactivity ratios and its significance, kinetics, different copolymers, random, alternating, azeotropic copolymerization, block and graft copolymers, techniques for copolymerization-bulk, solution, suspension, emulsion.

Polymer Characterization: Solubility and swelling, concept of average molecular weight, determination of number average, weight average, viscosity average and Z-average molecular weights, polymer crystallinity, analysis of polymers using IR, XRD, thermal (DSC, DMTA, TGA), microscopic (optical and electronic) techniques.

Synthesis and properties: Commodity and general purpose thermoplastics: PE, PP, PS, PVC, Polyesters, Acrylic, PU polymers. Engineering Plastics: Nylon, PC, PBT, PSU, PPO, ABS, Fluoropolymers Thermosetting polymers: PF, MF, UF, Epoxy, Unsaturated polyester, Alkyds. Natural and synthetic rubbers: Recovery of NR hydrocarbon from latex, SBR, Nitrile, CR, CSM, EPDM, IIR, BR, Silicone, TPE. Functional polymers: Photo responsive polymers, Ion conducting polymers, Piezoelectric polymers, Inorganic polymers.

Polymer blends and composites: Difference between blends and composites, their significance, choice of polymers for blending, blend miscibility-miscible and immiscible blends, thermodynamics, phase morphology, polymer alloys, polymer eutectics, plastic-plastic, rubber-plastic and rubber-rubber blends, Polymer composite systems: Types of composites, reinforced thermoplastic, thermoset, elastomer - resins FRP, particulate, long and short fibre reinforced composites.

Polymer Technology: Polymer compounding-need and significance, Additives for Plastics: Definition, classification, mechanism of action, method of incorporation of: fillers, plasticizer, stabilizer, (antioxidants/ozonants) Colorants, cross linking agents, blowing agents, antistatic agents, coupling agents, flame retardants, antiblock agents,

Polymer Rheology: Flow of Newtonian and non-Newtonian fluids, Nature of materials pseudoplastics, dilatants, Bingham plastic, Rheopexy and thixotropy, dependence of shear modulus on temperature, molecular/segmental deformations at different zones and transitions. Measurements of rheological parameters by capillary rotating, parallel plate,

cone-plate rheometer, viscoelasticity-creep and stress relaxations, mechanical models, control of rheological characteristics through compounding, rubber curing in parallel plate viscometer, ODR and MDR.

Polymer processing: Compression molding, transfer molding, injection molding, blow molding, reaction injection molding, extrusion, pultrusion, calendaring, rotational molding, thermoforming, rubber processing in two-roll mill, internal mixer.

Polymer testing: Mechanical-static and dynamic tensile, flexural, compressive, abrasion, endurance, fatigue, hardness, tear, resilience, impact, toughness. Conductivity-thermal and electrical, dielectric constant, dissipation factor, power factor, electric resistance, surface resistivity, volume resistivity, swelling, ageing resistance, environmental stress cracking resistance. Optical properties (gloss, clarity), Chemical properties (solubility, flammability, LOI, Vicat softening point & HDT, permeability, ageing & weathering, ESC, adhesion) flow properties (MFI, viscosity).

B. Chemistry Background:

Physical Chemistry:

[1] Basic principles and techniques of Quantum chemistry; postulates of quantum mechanics and Schrodinger equation, particle in one dimension, two dimension and three dimension box, degeneracy, Harmonic oscillator, rigid rotator and Hydrogen atom, angular momentum, shape of orbitals, spin-orbit coupling.

[2] Basic principles and applications of spectroscopy: rotational, vibrational, electronic, Raman, ESR, NMR.

[3] Chemical Kinetics: Rates of chemical reactions, Arrhenius equation, theory of reaction rates: collision and transition state theory, elementary, consecutive, and parallel reaction: steady state approximation, concept of catalyst.

[4]Chemical Equilibria and Thermodynamics: First, second, and third law of thermodynamics; entropy, free energy, partial molar quantities.

Inorganic Chemistry:

[1] Chemistry of main group elements: General characteristics, synthesis, structure and properties of their halides and oxides, polymorphism of carbon, phosphorous and sulphur. Synthesis, structure and properties of boranes, carboranes, borazines, phosphazenes, silicones. Interhalogens and noble gas compounds.

[2] Transition elements and coordination compounds: general characteristic of d and f block elements, coordination chemistry: structure, isomerism, bonding theories (VBT, CFT and LFT), reaction mechanism (substitution and electron transfer reaction), electronic spectra, magnetic properties, spectral and magnetic properties of lanthanides and actinides complexes.

[3] Organometallic compounds and Bioinorganic: Metal carbonyls, metallocenes, use of organometallic compounds as catalyst in organic synthesis and homogeneous catalytic reactions; hydrogenation hydroformylation. Bioinorganic chemistry of Fe, Zn, Cu, Co and Mo.

Organic chemistry:

[1] Stereochemistry and Aromaticity: Chirality of organic molecules with or without chiral centres, configuration, Asymmetric synthesis, enantio and diastereoselective synthesis, stereoselective and stereospecific synthesis, Conformational analysis of cyclic and acyclic compounds, geometrical isomerism, Aromaticity; concept of aromaticity and Huckel rule in annulenes, fullerenes.

[2]Reaction Mechanism and pericylic reactions: Name reactions; Favorski reaction, Michael addition, Ene reaction, Barton reaction, Shapiro reaction, Baeyer-Villiger reaction, Chichibabin reaction, reagents in organic synthesis; DDQ, LDA, selenium dioxide, metal hydride, Pericyclic reaction : Electrocyclic, cycloaddition and sigmatropic reaction, Orbital correlation, FMO and PMO treatments, Cope and Claisen rearrangements.

[3]Spectroscopy and Biomolecules: Principles and applications of UV-visible, IR, NMR and Mass spectroscopy in the structure elucidation of organic compounds, Biomolecules; structure and function of biopolymers such as carbohydrates, protein, nucleic acid, steroids, terpenoids and alkaloids.

C. Engineering Back ground:

Linear Algebra: Matrix algebra, Systems of linear equations, Eigen values and eigenvectors.

Calculus:
Functions of single variable, Limit, continuity and differentiability, Mean value theorems, Evaluation of definite and improper integrals, Partial derivatives, Total derivative, Maxima and minima, Gradient, Divergence and Curl, Vector dentities, Directional derivatives, Line, Surface and Volume integrals, Stokes, Gauss and Green's theorems.

Differential equations: First order equations (linear and nonlinear), Higher order linear differential equations with constant coefficients, Cauchy's and Euler's equations, Initial and boundary value problems, Laplace transforms, Solutions of one dimensional heat and wave equations and Laplace equation.

Complex variables: Analytic functions, Cauchy's integral theorem, Taylor and Laurent series, Residue theorem.

Probability and Statistics: Definitions of probability and sampling theorems, Conditional probability, Mean, median, mode and standard deviation, Random variables, Poisson, Normal and Binomial distributions.

Numerical Methods: Numerical solutions of linear and non-linear algebraic equations Integration by trapezoidal and Simpson's rule, single and multi-step methods for differential equations.

Chemical Engineering

Process Calculations and Thermodynamics: Laws of conservation of mass and energy; use of tie components; recycle, bypass and purge calculations; degree of freedom analysis. First and Second laws of thermodynamics. First law application to close and open systems. Second law and Entropy Thermodynamic properties of pure substances: equation of state and departure function, properties of mixtures: partial molar properties, fugacity, excess properties and activity coefficients; phase equilibria: predicting VLE of systems; chemical reaction equilibria.

Fluid Mechanics and Mechanical OperationsFluid statics, Newtonian and non-Newtonian fluids, Bernoulli equation, Macroscopic friction factors, energy balance, dimensional analysis, shell balances, flow through pipeline systems, flow meters, pumps and compressors, packed and fluidized beds, elementary boundary layer theory, size

reduction and size separation; free and hindered settling; centrifuge and cyclones; thickening and classification, filtration, mixing and agitation; conveying of solids.

Heat Transfer:Conduction, convection and radiation, heat transfer coefficients, steady and unsteady heat conduction, boiling, condensation and evaporation; types of heat exchangers and evaporators and their design.

Mass Transfer: Fick's laws, molecular diffusion in fluids, mass transfer coefficients, film, penetration and surface renewal theories; momentum, heat and mass transfer analogies; stagewise and continuous contacting and stage efficiencies; HTU & NTU concepts design and operation of equipment for distillation, absorption, leaching, liquid-liquid extraction, drying, humidification, dehumidification and adsorption.

Chemical Reaction Engineering: Theories of reaction rates; kinetics of homogeneous reactions, interpretation of kinetic data, single and multiple reactions in ideal reactors, non-ideal reactors; residence time distribution, single parameter model; non-isothermal reactors; kinetics of heterogeneous catalytic reactions; diffusion effects in catalysis.

Plant Design and Economics: Process design and sizing of chemical engineering equipment such as compressors, heat exchangers, multistage contactors; principles of process economics and cost estimation including total annualized cost, cost indexes, rate of return, payback period, discounted cash flow, optimization in design.

Chemical Technology: Inorganic chemical industries; sulfuric acid, NaOH, fertilizers (Ammonia, Urea, SSP and TSP); natural products industries (Pulp and Paper, Sugar, Oil, and Fats); petroleum refining and petrochemicals; polymerization industries; polyethylene, polypropylene, PVC and polyester synthetic fibers.

Instrumentation and Process Control: Measurement of process variables; sensors, transducers and their dynamics, transfer functions and dynamic responses of simple systems, process reaction curve, controller modes (P, PI, and PID); control valves; analysis of closed loop systems including stability, frequency response and controller tuning, cascade, feed forward control.