PRINCIPLES OF POLYMER SYNTHESIS

PROF. RAJAT K DAS
Materials Science Centre
IIT Kharagpur

INTENDED AUDIENCE : Chemistry, M.Tech

INDUSTRY SUPPORT : All industries where polymer and polymer products are being designed, developed and used

COURSE OUTLINE :

This course will introduce and discuss the basic principles of polymer chemistry. Specifically, it will stress upon the fundamentals of important polymerization reactions (emphasis on step polymerization and radical polymerization) and the principles that govern the structure of the resulting polymers. Synthesis and structure-property relation of several industrially important polymers will be discussed illustrating the applications of these principles. The course will also contain an introduction to basic chemical reactor design principles.

ABOUT INSTRUCTOR :

Prof. Rajat K. Das is an Assistant Professor at Materials Science Centre, IIT Kharagpur. His research interests include smart stimuli responsive polymeric materials and multiple network hydrogels. He is taking the course ‘Manufacture of Industrial Polymers’ for 1st year MTech students of the centre.

COURSE PLAN :

Week 1: Historical development of polymer science (since the early 0th century), classification of polymers (based upon the structure of polymers/based upon mechanism of polymerization), concept of average molecular weight of polymers, how to determine different averages for molecular weight (specific methods such as gel permeation chromatography, vapour pressure osmometry, viscosity measurement, membrane osmometry etc. will be discussed in some detail).

Week 2: Step polymerizationControl of molecular weight (stoichiometric excess or monofunctional impurity),number fraction and weight fraction distribution functions, side reactions in step polymerization (cyclization vs linear polymerization, the effect of ring stability and kinetic factor), interfacial polymerization (general principle along with specific examples, applicability).

Week 3: Chain polymerizationgeneral discussion of radical vs ionic polymerization; types of initiators; rate expression for radical chain polymerization, initiator efficiency; different modes of termination (coupling and disproportionation), chain transfer reactions and molecular weight control, autoacceleration, ceiling temperature.

Week 4: Chain polymerization (contd..)Effect of temperature on rate of radical chain polymerization and on molecular weight of polymers, dead end polymerization; Chain copolymerizationterminal model and derivation of instantaneous copolymer composition, concept of reactivity ratio, ideal copolymerization, alternating and azeotropic copolymerization, copolymer composition drift with conversion, experimental determination of reactivity ratio, microstructure of copolymers; Living polymerization methods such as ATRP, NMD, and RAFT. Discussion of examples from research papers that utilize some of these strategies to obtain specific properties.

Week 5: Design of Chemical ReactorsDifferent kinds of reactors (batch, CSTR, PFR, PBR etc.), basic mole balance equations and concept of reactor design with respect to the desired outcome of a chemical reaction (sizing of CSTR and PFR with respect to a targeted conversion in steady state), PFRs in series vs CSTRs in series.

Week 6: Design of Chemical Reactors (contd..)Effect of the reactor on the molecular weight distribution in polymerization (radical vs step growth), Selectivity in chemical reaction vs choice of reactor, basic energy balance equation, multiplicity of steady states in CSTR, ignition and extinction temperature, application of these concepts in polymerization.

Week 7: Industrial synthesis and structure-property relation of important engineering step polymers and specialty polymers (+)

Week 8: Industrial synthesis and structure-property relation of important engineering step polymers and specialty polymers (+ polyesters, polycarbonates, epoxy resins, aliphatic and aromatic polyamides, polyurethanes, polyimides etc.); different fiber spinning processes