

## **PROF. SHISHIR SINHA**

Department of Chemical Engineering IIT Roorkee

**INTENDED AUDIENCE :** Chemical engineering, polymer engineering, polymer technology, mechanical engineering

**INDUSTRIES APPLICABLE TO :** Useful for all polymer industries and companies related to surface and interfacial technology such as plastic, paints, rubber, resin, adhesive, and advanced polymeric material industries.Reliance Industries Limited ;GAIL India Limited and many more

## COURSE OUTLINE :

The course provide a complete overview of current and future aspects in polymer engineering. The finished polymer product properties are usually determined during the production process and hence it very essential to understand all the fundamentals and chemistry behind the polymerization process. Various terms such as reaction initiation, propagation, termination, reaction kinetics, thermal kinetics, molecular weight, and physical features such as microstructures, morphology, tensile and fractural strength etc. will be discussed in this course. The general polymerization concepts, principles, kinetics and methodology will be discussed through various examples. The course will be helpful for polymer and chemical engineer, students and industries for the advancement in the concepts related to polymer reaction engineering.

## ABOUT INSTRUCTOR :

Prof.Shishir Sinha is presently working as Professor and Head in the Department of Chemical Engineering at IIT Roorkee. He has been teaching the courses related to Process Utilities and Safety, Chemical Engineering Thermodynamics and safe Operation to Petroleum industries to undergraduate and postgraduate students for more than 12 years.

## COURSE PLAN :

**Week 1:** Introduction to polymerization process: classification of polymers, Short history, monomer and its distribution, Polymer and its composition, Isomerism in polymers

**Week 2 :** Bonding forces in polymers, Molecular weight and its distribution, control of polymer synthesis; thermodynamic and kinetic control, diffusion control, polymer end chain control & polymerization process, control strategies

**Week 3 :** Morphology of polymers, Introduction to reactor design, Interpretation of batch reactor data; Rate equations, Kinetic equations for unimolecular irreversible different order reaction such as Zero order, first order

Week 4 : Interpretation of batch reactor data; Kinetic equations for unimolecular & bimolecular irreversible different order reaction such as second order& nth order, Half -life, varying and constant volume reaction system, Design equations for ideal reactors, namely batch, CSTR, plug flow, design equation for single reaction systems using batch and semi batch, CSTR, PFR, Multiple reactor system; reactor in series and parallel, Preference of type of reactor used, Best arrangement in ideal reactors

**Week 5 :** Recycle reactor, Auto catalytic reactions, Design for multiple reactions: Parallel and series reactions, quantitative and qualitative treatment of product distribution and of reactor size for different types of ideal reactors, selectivity and yield, reactors in series and parallel for single reaction system, related problems

**Week 6 :** Problems; related to reaction kinetics, series and parallel reaction and multiple reactor systems, Reaction engineering of step growth polymerization:Basic properties & Examples of commercially important polymers, Reactivity of functional groups Kinetics of step polymerization, Self-Catalyzed Polymerization, External Catalysis of Polymerization,Effect of Nonequivalence of Functional Groups, Accessibility of functional groups, Equilibrium considerations, Cyclization versus linear polymerization

**Week 7**: Step growth polymerization; Molecular weight control in linear polymerization, Molecular weight distribution in linear & non-linear polymerization, Introduction to radical chain polymerization, Basic concepts of resonance, Comparison between radical and step polymerization, Comparison between radical and ionic chain polymerization, Thermodynamic and kinetic aspect of Radical Chain Polymerization, Effect of Substituents, Modes of Propagation of Monomer Units, Experimental Facts from Literature, Synthesis of Head-to-Head Polymers, Polymerization Sequence: Initiation, Propagation, Termination

**Week 8 :** Radical chain polymerization; Rate Expression, Cage Efficiency, Determination of Rate of polymerization, Precipitation of Polymer, Polymer and Process Analysis for polymerization, Initiation, Stability and Half Life of Initiators, Dependence of Polymerization Rate on Initiator, Dependence on Monomer, Initiation in aqueous media,

**Week 9 :** Redox Initiation (cont.), Initiation in non-aqueous media,Rate of Redox polymerization, Photochemical Initiation

Photosensitizer, Mechanism of Photo-initiation, Rate of Photo-polymerization, Absorbed light Measurement, Initiation by Ionizing Radiation, Other initiation techniques, Electrolytic polymerization, Plasma polymerization, Sonication, Kinetic Chain Length and other important terms, Heterogenous Polymerization: Precipitation, Suspension

**Week 10**: Heterogenous Polymerization: Precipitation, Suspension (cont.) & Emulsion Polymerization; microstructural feature, factors affecting the emulsion polymerization, process of emulsion polymerization, mechanism kinetic and thermodynamics, Model, surface active agents, process, population balance, Physical properties and phase equilibrium calculations

**Week 11 :** Emulsion Polymerization; particle nucleation, morphology, types of reactors used for emulsion polymerization, performance of emulsion, polymerization reactors, Population balance, Implementation of emulsion polymerization, Ionic Chain Polymerization: Comparison between radical and ionic chain polymerization, Living and Dormant polymers and polymerizability

**Week 12 :** Ionic Chain Polymerization: classification of ionic species, effect of solvents, conductance studies, initiation and propagation in ionic polymerization, effect of solvating agent, Heat and Entropy of dissociation of ionic pairs, types of ions, cationic polymerization, Chain