Polymer Reaction Engineering

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European credits ECTS: 5

Teaching Language: English

Supporting files: English

	Number of course slots (1h)	Number of course slots (1h)
Magisterial	36	
Problem based learning (PBL)	14	

Description

- Advanced concepts of polymerization reaction engineering are pursued in this course. Especially non-linear polymers (and the main mechanisms leading to branched and croslinked polymers) are addressed in the modeling of the most used polymerization techniques (coordination and free-radical polymerization)
- Emulsion polymerization and related disperse phase polymerization techniques are studied in detail.

Outline

Part 1: Introduction to polymerization reactors and polymer reaction engineering
Microstructural features of polymers and their effect on properties
Classes of polymerizations
Polymerization techniques
Main commercial polymers

Part 2: Coordination polymerization
Polymerization kinetics for multiple site catalysts
- Copolymerization
- Long-chain branching

Inter- and intraparticle mass and heat transfer
- Particle fragmentation and morphology control
- Single particle models: inter- and intraparticle mass and heat transfer

Part 3: Free-radical polymerization: Homogeneous systems
Free radical polymerization mechanism and kinetics: non-linear polymers
Inter- intramolecular chain transfer to polymer

Propagation to pendant double bond
β-scission
Crosslinking reactions
Kinetic and population balances for modeling MWD in non-linear polymers

- The method of the moments and its limitations

Copolymerization in batch and semibatch reactors

- Monomer Feeding Strategies

Part 4: Free-radical polymerization: Heterogeneous systems

Introduction
High-impact polystyrene (HIPS)
Polyvinylchloride (PVC) bulk polymerization

Part 5 : Emulsion polymerization

Introduction: Review of physical description and compartmentalization importance
Kinetics of emulsion polymerization

- Polymerization rate
- Average number of radicals per particle, $\bar{n}$: entry, exit and termination
- Monomer partitioning in different phases

Stability of polymer colloids: DLVO theory
Particle nucleation: homogeneous, heterogeneous and coagulative
Modeling molar mass distribution: pragmatic approaches
Related processes:

- Inverse emulsion polymerization
- Miniemulsion polymerization
- Microemulsion polymerization
- Dispersion polymerization

Part 6: Step-growth polymerization

Polymerization kinetics and modeling
Industrial step-growth products

- PET production process and modeling

Problem based learning (PBL)

Part 3 is taught using a *Problem based learning* methodology where the students learn the fundamentals of free-radical homo and copolymerization in batch and semibatch reactors using a simulation software package (Predici©) to understand the effect of important mechanisms and process variables in the properties of the (co)polymers (composition and molar mass distribution).