# 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).