INSTITUTO POLITÉCNICO DE BRAGANÇA

Course Unit	Polymer Reaction Engineering			Field of study	Polymers		
Master in	Chemical Engineering			School	School of Technology and Management		
Academic Year	2019/2020	Year of study	1	Level	2-1	ECTS credits	6.0
Type	Semestral	Semester	2	Code	6362-354-1201-00-19		

Workload (hours)	162	Contact hours	T	TP	PL	TC	S	E	OT	O
			30	-	30	-	-	-	-	-

T - Lectures; TP - Lectures and problem-solving; PL - Problem-solving, project or laboratory; TC - Fieldwork; S - Seminar; E - Placement; OT - Tuturial; O - Other

Name(s) of lecturer(s): Rolando Carlos Pereira Simões Dias

Learning outcomes and competences

At the end of the course unit the learner is expected to be able to:
1. Identify and distinguish the main different kinds of industrial polymerization reactors.
2. Identify the main kinds of linear polymers synthesized by polycondensation and use the associated calculation techniques.
3. Identify linear polymers that can be synthesized by ionic polyaddition and use the associated calculation techniques.
4. Recognize industrially relevant classes of polymers synthesized through radical homo or copolymerizations and use the associated calculation techniques.
5. Recognize the importance of branching and quantify this phenomenon in some industrially important polymers.
6. Apply MATLAB in the numerical resolution of polymerization reaction engineering problems, namely considering initial value problems (IVP) and boundary value problems (BVP).

Prerequisites

Before the course unit the learner is expected to be able to:
1. Demonstrate knowledge on chemical reactors.
2. Demonstrate knowledge on chemical kinetics.
3. Establish and solve conservation laws.

Course contents

Historical notes and importance of polymer industry nowadays. Introduction to polymerization reactors and properties of the resulting polymers. Linear polycondensations. Linear ionic polyadditions. Linear radical polyadditions. Linear radical copolymerizations. Non linear polymerizations. Controlled radical polymerization. The course includes also experimental work concerning the polymer synthesis, their characterization and application.

Course contents (extended version)

1. Historical notes and importance of polymer industry nowadays
   - Natural polymers used before 1800
   - Beginning of the production of synthetic polymers
   - Examples of polymers with industrial relevance
2. Introduction to polymerization reactors and properties of the resulting polymers
   - Solution polymerization
   - Bulk polymerization
   - Suspension polymerization
   - Emulsion polymerization
   - Chain length distribution and molecular weight distribution
   - Sequence length distribution
   - Average radius of gyration
3. Linear polycondensations
   - Linear polycondensation of an AB monomer
   - Schulz-Flory distribution
   - Linear polycondensation of A2+B2 monomers
4. Linear ionic polyadditions
   - Ideal ionic polyaddition
   - Moment generating functions
   - Poisson distribution
5. Linear radical polyadditions
   - Initiation, propagation, termination and chain transfer reactions
   - Pseudo steady-state of radical concentration and other simplifying assumptions
   - Dead polymer
   - Kinetic models and influence of the kinetic mechanisms on the chain length distribution
6. Linear radical copolymerizations
   - Copolymer composition in radical polymerizations
   - Mayo-Lewis equation
   - Influence of the reactivity ratios
   - Sequence length distribution in radical copolymerizations
7. Non linear polymerizations
   - Non linear polycondensation of an Af monomer
   - Gel point
   - Stockmayer distribution
   - Weight fraction of sol
   - Non linear polycondensation of A3+B2 monomers
   - Influence of the monomer molar ratio
   - Non-linear radical and ionic polymerizations
8. Controlled Radical Polymerization (CRP)
   - Advantages of CRP comparatively to conventional radical polymerization
   - Calculation case study with ATRP
   - Kinetic modeling of CRP systems

Recommended reading

1. Polymer Reaction Engineering, J. Asua, Wiley-Blackwell, 2007
2. Handbook of Polymer Reaction Engineering, T. Meyer, J. Keurentjes, Wiley-VCH, 2005
3. Polymerization Process Modeling, N. A. Dotson, R. Galván, R. L. Laurence, M. Tirrell, Wiley-VCH, 1996
4. Modeling and Simulation in Polymer Reaction Engineering: A Modular Approach 1st Edition, Klaus-Dieter Hungenberg, Michael Wulkow, Wiley-VCH, 2018
5. Elementos de Engenharia das Reações de Polimerização, Rolando Dias, ESTIG, IPB, 2019

Teaching and learning methods

The unit will be taught using a combination of lectures, self guided learning and practice classes. Students will be provided with a study guide and support material, including e-learning facilities.

Assessment methods

1. Alternative 1 - (Regular, Student Worker) (Final, Supplementary, Special)
   - Development Topics - 30% (Includes experimental work)
   - Presentations - 10% (Includes the presentation of the experimental work performed)
   - Final Written Exam - 60%
2. Alternative 2 - (Regular, Student Worker) (Special)
   - Final Written Exam - 100%
3. Alternative 3 - (Student Worker) (Final, Supplementary)
   - Final Written Exam - 100%

Language of instruction

English

Electronic validation

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22-02-2020	23-02-2020	23-02-2020	28-03-2020