INSTITUTO POLITÉCNICO DE BRAGANÇA

Course Unit	Engineering and Molecular Architecture of Polymers	Field of study	Polymers
Master in	Chemical Engineering	School	School of Technology and Management
Academic Year	2023/2024	Year of study	1
Level	2-1	ECTS credits	6.0
Type	Semestral	Semester	2
Code	6362-756-1201-00-23		

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

T - Lectures; TP - Lectures and problem-solving; PL - Problem-solving, project or laboratory; TC - Fieldwork; S - Seminar; E - Placement; OT - Tutorial; 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 different routes allowing the control and tailoring of the molecular architecture of polymers, namely based on alternative mechanisms for synthesis/modification.
2. Identify polymerization mechanims by polycondensation, ionic polyaddition, linear/non-linear radical polymerization or controlled radical polymerization (RAFT, ATRP, NMRP).
3. Develop in MATLAB calculation tools for the designing of the molecular architecture of polymers based on the polymer reaction engineering and kinetic mechanisms intervenient in formation processes.
4. Recognize different routes for the functionalization and natural-synthetic hybridization of polymers and their present applications in engineering.
5. Identify applications of tailored polymers in energy conversion/storage and biotechnology.
6. Identify applications of tailored polymers in biomedicine; virus targeting; molecular recognition; adsorbents or cancer diagnosis/treatment.

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

Polycondensation; Ionic polyadditions; Radical polyadditions; Non-linear polymerization; RAFT; ATRP; NMRP; Moment generating functions; MATLAB calculations; Degree of polymerization; Schulz-Flory and Poisson distributions; Functionalization; Hybrid synthetic-natural; Functionalization of polymer networks; Case studies in engineering; energy conversion/storage; Biotechnology; Biomedicine; Glycopolymers; Virus targeting; Molecular imprinting; Tailored adsorbents; Cancer diagnosis and treatment.

Course contents (extended version)

1. Linear polycondensation
   - Linear polycondensation of AB monomers, Schulz-Flory distribution. MATLAB calculations.
   - Linear polycondensation of A2+B2 monomers. MATLAB calculations.
   - Designing of polyamides, polyesters, polyurethanes and other linear polycondensation polymers.
   - Sequence size distributions.
   - Applications of tailored linear polycondensation polymers in engineering and biomedicine.
2. Linear ionic polyadditions
   - ideal ionic polyaddition, moment generating functions, Poisson distribution. MATLAB calculations.
   - Ionic polymerization of vinyl monomers and control of the molecular architecture of the products.
   - Tailoring the degree of polymerization, block copolymers. MATLAB calculations.
   - Applications of functionalized ionic polymers in engineering, biotechnology and biomedicine.
3. Linear radical polyadditions
   - Initiation, propagation, termination and chain transfer reactions.
   - Pseudo steady-state of radical concentration and other simplifying assumptions.
   - Dead polymer. Kinetic models.
   - Influence of the kinetic mechanisms on the chain length distribution.
   - The method of the moments. MATLAB calculations with stiff systems of differential equations.
   - Radical polymerization with the tailoring and synthesis of hybrid synthetic-natural materials.
4. Linear radical copolymerization
   - Copolymer composition in radical polymerizations.
   - Mayo-Lewis equation, influence of the reactivity ratios.
   - Tailoring of sequence chain length distributions in radical copolymerizations.
   - Functional polymers via free radical copolymerizations. Stimuli-responsive polymers.
   - MATLAB calculations with stiff systems of differential equations.
   - Application of copolymers in engineering, biotechnology and biomedicine.
5. Non-linear polymerization
   - Non-linear polycondensation of Af monomers, 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.
   - Calculation methods in MATLAB based on moment generating functions.
   - Tailoring and functionalization of polymer networks and gels, radius of gyration.
   - Polymer networks and gels in engineering, energy storage, biotechnology and biomedicine.
6. Reversible addition-fragmentation chain-transfer (RAFT) polymerization
   - Reversible deactivation-radical polymerization with different kinds of RAFT agents.
   - The RAFT kinetic scheme. Aqueous RAFT polymerization.
   - MATLAB calculations with stiff systems of differential equations.
   - Linear and non-linear RAFT polymerization using the method of the moments. MATLAB calculations.
   - Control of molecular architecture and functionalization with RAFT polymerization.
   - Applications with glycopolymers for virus targeting.
   - Molecular imprinting with RAFT polymerization. Applications with diagnosis and cancer treatment.
7. Atom Transfer Radical Polymerization (ATRP)
   - Typical chemical systems for ATRP. The ATRP kinetic scheme. Organic and aqueous ATRP polymerization.
   - MATLAB calculations with stiff systems of differential equations for ATRP.
   - Linear and non-linear ATRP using the method of the moments. MATLAB calculations.
   - Control of molecular architecture and functionalization with ATRP.
   - Hybrid synthetic-natural polymers through ATRP.
   - Molecular imprinting with ATRP. Applications with tailoring of adsorbents.
   - Applications for chemical industries and for biotechnology.
   - Applications in energy storage and with cancer diagnosis/treatment.

Course contents (extended version)

8. Nitroxide-Mediated Radical Polymerization (NMRP)
   - Typical chemical systems for NMRP. Alkoxy amine compounds in NMRP.
   - Grafting with NMRP. The NMRP kinetic scheme.
   - MATLAB calculations with stiff systems of differential equations in NMRP.
   - Linear and non-linear NMRP polymerization using the method of the moments.
   - Control of molecular architecture and functionalization with NMRP.
   - Hybrid synthetic-natural polymers through NMRP.
   - Bio-conjugation (e. g. polymer-peptide conjugates) with NMRP.
   - Applications with sugar sensors/receptors and other biomedical applications.

Recommended reading

1. Principles of Polymerization, George Odian, Fourth Edition, Wiley-Interscience, 2004
2. Modeling and Simulation in Polymer Reaction Engineering: A Modular Approach 1st Edition, Klaus-Dieter Hungenberg, Michael Wulkow, Wiley-VCH, 2018
3. Polymeric Nanosystems, Theranostic Nanosystems, Volume 1, Md Saquib Hasnain, Amit Nayak, Tejraj Aminabhavi, Elsevier, 2023
4. Sustainable Hydrogels, Synthesis, Properties, and Applications, Sabu Thomas, Bhasha Sharma, Purnima Jain, Shashank Shekhar, Elsevier, 2023
5. Systems of Nanovesicular Drug Delivery, Amit Nayak, Md Saquib Hasnain, Tejraj Aminabhavi, Vladimir Torchilin, Elsevier, 2022

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. Specific case studies are analysed at laboratory.

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

Rolando Carlos Pereira Simões Dias	Hélder Teixeira Gomes	Simão Pedro de Almeida Pinho	José Carlos Rufino Amaro
12-02-2024	13-03-2024	13-03-2024	16-03-2024