

Course Unit	Chemical Reaction Engineering		Field of study	Chemical Process Engineering	
Bachelor in	Chemical Engineering		School	School of Technology and Management	
Academic Year	2023/2024	Year of study	2	Level	1-2
Type	Semestral	Semester	2	ECTS credits	6.0
			Code	9125-755-2202-00-23	
Workload (hours)	162	Contact hours	T 30	TP -	PL 30
			TC -	S -	E -
			OT -	O -	

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) Paulo Miguel Pereira de Brito, Mónia Andreia Rodrigues Martins

### Learning outcomes and competences

At the end of the course unit the learner is expected to be able to:

1. Remember the chemical kinetics fundamentals.
2. Analyse experimental data in order to estimate reaction kinetics models.
3. Understand and design ideal reactors.
4. Analyse and design ideal reactors net configurations.
5. Analyse and design multiple stoichiometric reactions.
6. Analyse and design non-isothermal reactors.

### Prerequisites

Before the course unit the learner is expected to be able to:

1. Reveal knowledge acquired by the study of Engineering ground sciences, Physics and Mathematics.
2. Reveal knowledge of Engineering sciences fundamentals, namely in the field of chemical kinetics.
3. Have experience in using computational tools.

### Course contents

1. Introduction to chemical reaction engineering. 2. Kinetics of homogeneous reactions. 3. Batch reactor: experimental data analysis. 4. Ideal reactors. 5. Ideal reactors design. 6. Multiple stoichiometry design. 7. Non-isothermal reactors.

### Course contents (extended version)

1. Introduction to Chemical Reaction Engineering.
  - Objectives of Chemical Reaction Engineering curricular unit.
  - Chemical reactors' classification.
  - Design equations.
  - Chemical reactions' classification.
2. Homogeneous reactions chemical kinetics.
  - Equations to quantify reaction velocity.
  - Molecularity. Reaction order. Elementar reaction.
  - Reaction velocity.
  - Arrhenius law.
3. Batch reactor.
  - The conversion concept.
  - Analysis of experimental data: integral and differential methods.
  - Steady volume batch reactors.
  - Irreversible first and second order reactions. Reactions of order n. Reactions of zero order.
  - Irreversible parallel and serial reactions.
  - Reversible one order reactions.
  - Variable order reactions.
  - Variable volume batch reactor.
4. Ideal reactors
  - Material balances and design equations.
  - Batch and flux reactors.
  - Continuous and discontinuous operations. Steady-state and transient operations.
  - Residence time in flux reactors.
  - Perfectly stirred and plug-flow reactors.
5. Ideal reactors design.
  - Comparison of performance for different types of ideal reactors.
  - Serial and/or parallel configurations of ideal reactors.
  - Continuously stirred reactors in series. Different types of reactors in series.
  - Introduction of recycle currents in plug-flow reactors systems.
6. Multiple stoichiometric reactions.
  - Desired product and by-products rates.
  - Relative yield and selectivity: integral and differential definitions.
  - Parallel and serial reactions: plug-flow and perfectly mixed reactors.
  - Operational optimisation.
7. Non-isothermal reactors.
  - Van't Hoff equation.
  - Optimal temperature for isothermal operation.
  - Optimal progression of temperatures.
  - Ideal reactor design for optimal progression of temperatures operations.

### Recommended reading

1. O. Levenspiel, Chemical Reaction Engineering, 3rd edition, John Wiley & Sons (1998)
2. J. Villermaux, Génie de la Réaction Chimique. Conception et Fonctionnement des Réacteurs, Technique & Documentation, Lavoisier (1982)
3. S. Fogler, Elements of Chemical Reaction Engineering, 3rd edition, Prentice-Hall (1998)
4. F. Lemos, J. Madeira Lopes, F. Ramôa Ribeiro, Reactores Químicos, IST Press (2002)

### Teaching and learning methods

Theoretical classes: Chemical reaction engineering and kinetics fundamentals exposition, analysis and discussion. Practical classes: Tutored solution of problems and case-studies. Non-presential work: Individual and group study, bibliography analysis, problems solution.

Assessment methods

1. Alternative 1 - (Regular, Student Worker) (Final)

- Practical Work - 20%

- Intermediate Written Test - 80% (2 tests; minimum test average: 7. 0 (in 20))

2. Alternative 2 - (Regular, Student Worker) (Final)

- Practical Work - 20%

- Final Written Exam - 80% (Minimum grade: 7. 0 (in 20))

3. Alternative 3 - (Regular, Student Worker) (Supplementary, Special)

- Final Written Exam - 100%

Language of instruction

English

Electronic validation			
Paulo Miguel Pereira de Brito	Hélder Teixeira Gomes	António Manuel Esteves Ribeiro	José Carlos Rufino Amaro
13-02-2024	13-03-2024	13-03-2024	16-03-2024