

Course Unit	Chemical Process Optimization	Field of study	Process Simulation, Control and Optimization
Master in	Chemical Engineering	School	School of Technology and Management
Academic Year	2023/2024	Year of study	1
Type	Semestral	Semester	2
Level	2-1	ECTS credits	6.0
Code	6362-756-1202-00-23		
Workload (hours)	162	Contact hours	T 15 TP - PL 45 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

### Learning outcomes and competences

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

1. Understand the importance of optimisation as the final stage in the chemical processes design strategy.
2. Know the basic features that characterise the optimisation mathematical models.
3. Know the mathematical principles in which the main non-linear non-restrained optimisation numerical solution methods are based.
4. Understand the formulation and solution of typical linear programming models.
5. Understand the main solution methods for non-linear programming models.
6. Select the most suitable solution method for a particular optimisation problem and use commercial software for its application.
7. Understand the importance of the integration concept in Chemical Processes design.
8. Know the fundamentals of the heat integration procedure through pinch analysis application and understand its potential extension to other types of integration.

### Prerequisites

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

1. Reveal knowledge acquired by the study of Engineering ground sciences.
2. Reveal knowledge of Engineering Sciences fundamentals.
3. Evidence experience in the use of computational tools.

### Course contents

1. Introduction to optimisation and integration of Chemical Processes.
2. Basic concepts of mathematical optimisation.
3. Non-restrained non-linear optimisation.
4. Linear programming.
5. Non-linear programming.
6. Design and analysis of experiments.

### Course contents (extended version)

1. Introduction.
  - The importance of chemical process optimisation and integration.
  - Modelling and objective functions formulation.
  - The optimisation tree.
2. Basic concepts.
  - Concept of optimal of an one or a multidimension function.
  - Analytical approaches for the optimisation of one- and multidimension functions.
3. Non-restrained non-linear optimisation.
  - Formulation of non-linear non-restrained multidimension optimisation problems.
  - Numerical methods for non-linear optimisation.
4. Linear programming.
  - Formulation of linear restrained optimisation problems (Linear Programming).
  - Solution methods for linear programs: primal simplex algorithm in the table form.
  - Mixed integer linear programming: Branch-and-Bound method.
5. Non-linear programming.
  - Formulation of non-linear restrained optimisation problems (Non-Linear Programming).
  - Solution methods for non-linear programs: Kuhn-Tucker conditions, SLP e SQP.
6. Design and analysis of experiments.
  - Introduction, concepts. The analysis of variance. Factorial designs.
  - Experiments with a single factor: complete factorial design and fractional factorial design.
  - Factorials 2k and 3k.
  - Response Surface Methodology.

### Recommended reading

1. T. F. Edgar, D. M. Himmelblau, L. S. Lasdon, Optimization of Chemical Processes, 2nd edition, McGraw-Hill (2001)
2. M. Ramalheite, J. Guerreiro, A. Magalhães, Programação Linear, Volume I, McGraw-Hill (1985)
3. D. C. Montgomery, Design and Analysis of Experiments, 10th ed. , John Wiley & Sons (2019)
4. R. H. Myers, D. C. Montgomery, C. M. Anderson-Cook, Response Surface Methodology: Process and Product Optimization Using Designed Experiments, 4th Edition, John Wiley & Sons (2016)

### Teaching and learning methods

Theoretical Classes: Optimisation and integration techniques analysis and discussion with case-studies solution application. Practical Classes: Tutored solution of application problems and case-studies. Non-presential work: Individual and group study, bibliography reading, problem solution and essays writing.

### Assessment methods

1. Alternative 1 - (Regular, Student Worker) (Final, Supplementary)
  - Intermediate Written Test - 20% (Partial Exam.)
  - Final Written Exam - 30% (Global Exam.)
  - Case Studies - 30% (Formulation and solution of problems relating to case-studies in Chemical Processes.)
  - Practical Work - 20% (Solution of problems in the classroom.)
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

Paulo Miguel Pereira de Brito	Hélder Teixeira Gomes	Simão Pedro de Almeida Pinho	José Carlos Rufino Amaro
13-02-2024	13-03-2024	13-03-2024	16-03-2024