INSTITUTO POLITÉCNICO DE BRAGANÇA

Course Unit	Chemical Process Simulation			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	Level	2-1	ECTS credits	6.0
Type	Semestral	Semester	2	Code	6362-756-1204-00-23		

Workload (hours)	162	Contact hours	T	TP	PL	TC	S	E	OT	O
			15	-	45	-	-	-	-	-

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): Hélder Teixeira Gomes

Learning outcomes and competences

At the end of the course unit the learner is expected to be able to:
1. Interpret processes data and recognize software used in the modelling and simulation of chemical processes
2. Demonstrate knowledge about process diagrams, process variables and degrees of freedom analysis. Recall the balance components
3. Develop dynamic and steady-state process models
4. Apply informatic tools of general use in the resolution of modelling and simulation problems in chemical engineering
5. Apply commercial simulation software in the resolution of chemical engineering simulation problems involving reaction
6. Apply commercial simulation software to simulate and analyse processes involving separations
7. Apply commercial simulation software to simulate, analyse and optimize chemical engineering processes

Prerequisites

Before the course unit the learner is expected to be able to:
1. Demonstrate strong knowledge on engineering and speciality science fundamentals
2. Demonstrate strong knowledge on mass and energy balances
3. Demonstrate strong knowledge on optimization methods
4. Demonstrate strong knowledge on the use of informatic tools

Course contents

Importance and potentialities of the modeling and simulation of chemical engineering processes. Identification of software used in the modeling and simulation of chemical processes. Application of general use software in the resolution of modeling and simulation of chemical engineering problems. Application of commercial software in the simulation, analysis and optimization of chemical engineering processes.

Course contents (extended version)

1. Introduction
   - The importance and potentialities of the modeling and simulation of chemical engineering processes
   - Software used in the simulation of chemical processes
2. Basic concepts
   - Modeling fundamentals: general aspects and modeling procedures in chemical engineering processes
   - Formulation of dynamic models: transient and steady states
   - Balance components: accumulation, convection, diffusion, interfacial transport, chemical reaction
   - Other relations/correlations needed in the modeling of chemical processes
   - Material balances
   - Energy balances
   - Momentum balances
   - Adimensionalization of variables
3. Modeling and simulation of chemical engineering processes
   - Simulation of processes described by partial differential equations
   - Modeling and simulation of tubular reactors
   - Plug-flow tubular reactor
   - Tubular reactor with axial dispersion
   - Energy balances in tubular reactors
4. Simulation of chemical engineering processes using commercial simulators
   - Process diagrams
   - Process variables
   - Mass, energy and momentum balances
   - Commercial simulators
   - Definition of thermodynamic properties and components package
   - Installation and definition of streams
   - Mixture processes
   - Reactors
   - Recycle and purge
   - Implementation of the Case Studies tool
5. Simulation of separation processes using commercial simulators
   - Separation columns
   - Simulation of a distillation column
   - Definition of specifications
   - Determination of temperature and composition profiles
   - Liquid-liquid extraction processes
   - Simple extractor
   - Multiple stage extraction processes
   - Extraction in column
   - Application of SET and ADJUST functions
6. Energetic integration and optimization in chemical processes using commercial simulators
   - Heat exchangers
   - Energy integration in distillation columns
   - Objective function and restrictions
   - Optimization methods
   - Implementation of the Optimizer function
   - Profit and production maximization

Recommended reading

1. W. D. Seider, J. D. Seader, D. R. Lewin, Product and Process Design Principles: Synthesis, Analysis and Evaluation, John Wiley & Sons, 2nd Edition, 2004

Recommended reading

2. C. A. Silebi, W. E. Schiesser, Dynamic Modeling of Transport Process Systems, Academic Press, 1992
3. J. Ingham, I. J. Dunn, E. Heinzle, J. E. Prenosil, Chemical Engineering Dynamics. An Introduction to Modeling and Computer Simulation, Wiley-VCH, 2nd Completely Revised Edition, 2000
4. R. G. E. Franks, Mathematical Modeling in Chemical Engineering, John Wiley & Sons, 1967

Teaching and learning methods

Theoretical-practical classes: exposition of modeling and simulation concepts and techniques, and of typical chemical engineering case studies. Practical classes: supervised resolution of modeling and simulation problems using computational tools. Non-contact period: study of subjects and resolution of chemical engineering modeling and simulation problems.

Assessment methods

1. Alternative 1 - (Regular, Student Worker) (Final)
   - Practical Work - 30%
   - Intermediate Written Test - 30%
   - Final Written Exam - 40%
2. Alternative 2 - (Regular, Student Worker) (Supplementary, Special)
   - Final Written Exam - 100%
3. Alternative 3 - (Student Worker) (Final, Supplementary, Special)
   - Final Written Exam - 100%

Language of instruction

English

Electronic validation

Hélder Teixeira Gomes	Simão Pedro de Almeida Pinho	José Carlos Rufino Amaro
01-03-2024	01-03-2024	02-03-2024