Proyecto/Guía docente de la asignatura

Course/ Asignatura	Chemical Process Analysis with Simulators / Análisis de Procesos Químicos con Simuladores		
Unit / Materia	Process Design / Diseño de Procesos		
Module / Módulo	Process & Product Engineering / Ingeniería de Procesos y Producto		
Degree / Titulación	Master in Chemical Engineering/ Máster en Ingeniería Química		
Plan Code / Plan	542	**Couse code/** Código	53749
Period/ Periodo de impartición	2nd Semester / 2º CUATRIMESTRE	**Type /** Tipo/Carácter	COMPULSORY / OBLIGATORIA
Level/Cycle / Nivel/Ciclo	MÁSTER	**Year** / Curso	1º
ECTS credits / Créditos ECTS	4.5 ECTS		
Language / Lengua en que se imparte	ENGLISH / INGLÉS		
Staff / Profesor/es responsable/s	LUIS VAQUERIZO MARTÍN ÁNGEL MARTÍN MARTÍNEZ		
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Department / Departamento	Ingeniería Química y Tecnología del Medio Ambiente		
Fecha de revisión por el Comité de Título	16/07/2024		

1. Location / Sense of the Subject

1.1 Contextualization

This subject is taught in the second semester of the first year of the Master's degree in Chemical Engineering. This is a very practical course in which students learn how to use commercial chemical process simulation software. The thermodynamic modelling of industrial processes and their dynamic simulation is studied in depth.

1.2 Relationship with other subjects

It is a continuation of the courses taught in the first semester, and a complement to those of second semester.

1.3 Prerequisites

2. Learning outcomes

2.1 Basic

CG02. Devise, project, calculate, and design processes, equipment, industrial facilities and services in the field of chemical engineering and related industrial sectors in terms of quality, safety, economy, rational and efficient use of natural resources, and environment preservation.

CG03. To lead and manage in a technical and economical way projects, facilities, plants, companies and technology centres in the field of chemical engineering and related industrial sectors.

CG04. Perform appropriate research, design and lead the development of engineering solutions, in new or uncertain environments, relating creativity, originality, innovation and technology transfer.

CG06. To be able to analyse and synthesize the continuous progress of products, processes, systems and services using criteria of safety, economic viability, quality and environmental management.

CG07. Integrate knowledge and face the complexity of making judgments and decision making, based on incomplete or limited information, including reflections on the social and ethical responsibilities of professional practice.

CG09. Communicate and discuss proposals and conclusions in multilingual, specialized and non-specialized forums, in a clear and unambiguous way.

CG10. Adapt to changes, being able to apply new and advanced technologies and other relevant developments, with initiative and entrepreneurial spirit.

CG11. To possess the abilities of the autonomous learning to maintain and to improve the own competences of the chemical engineering that allow the continuous development of the profession.

2.2 Specific

CEP03. Conceptualize engineering models, apply innovative methods in problem solving and use of suitable computer applications for the design, simulation, optimization and control of processes and systems.

CEP04. Ability to solve problems that are unfamiliar, incompletely defined, and have competing specifications, considering possible methods of solution, including the most innovative, selecting the most appropriate, and being able to correct the implementation, evaluating the different design solutions.

3. Aims

The general aim is to learn how to use the software tools available in the market to design, analyse and optimize processes in the chemical industry. To this end, three partial objectives are sequentially fulfilled:

- Learn how to develop steady state simulations, using HYSYS software.
- Learn how to transform steady state simulations into dynamic ones, using HYSYS.
- Use dynamic simulations to analyse and optimize continuous and batch processes.
- Learn to select, understand, evaluate, tune up and optimize the thermodynamic modelling of pure components and mixtures under specific operation conditions.

4. Contents

Workload in ECTS credits: 4.5

a. Contextualization and justification

(see section 1.1)

b. Learning objectives

(see section 3)

c. Syllabus

Unit 1: "Steady simulation with HYSYS"

1. **Introduction.** Practical case. Commercial software in chemical process simulation. HYSYS fundamentals. Help system.
2. **Using the Interface**
3. **Basic modelling.** Equilibrium Reactor. Attachments. Recycle. Databook. Distillation: Shortcut.
4. **Modelling tools**

Unit 2: "Dynamic simulation with HYSYS"

1. **Introduction**. Sample case: Propylene glycol reactor.
2. **Fundamentals of Chemical Processes Dynamic simulation with HYSYS**. General concepts. Holdup Model. Pressure-Flow Solver. General Guidelines.
3. **Moving from steady state to dynamic simulation**
4. **Scheduled operations**

Unit 3: "Thermodynamic modelling"

1. **Methods & Models**. Property Method. Phase Equilibrium Calculation. Property Method Selection. Properties calculation framework.
2. **Thermo Data Engine**. NIST Thermo Data Engine. Reference properties of pure components in database. Pure component estimation. Binary mixtures. Data evaluation. Data regression.
3. **Reliable Definition of New Components**. Automatic properties estimation. Reviewed properties estimation.

d. Teaching methods

(see section 5)

e. Workplan

Week 1: Start of Steady state section
Week 5: Assignment 1
Week 4: Start of Dynamic section
Week 11: Assignment 2
Week 10: Start of Properties section
Week 15: Assignment 3

f. Assessment

(see section 7)

g Training material

g.1 Basic Bibliography

- HYSYS Software User Guides (AspenTech).
- Aspen Properties Software User Guides (AspenTech).
- IVÁN DARÍO GIL: “Process Analysis and Simulation in Chemical Engineering”. 2016.

g.2 Additional Bibliography

g.3 Other telematic resources (knowledge pills, blogs, videos, digital magazines, mass courses (MOOC), ...)

The course Web page on Campus Virtual includes links to the videos with the theoretical contents of the subject. Access to the software is guaranteed for students enrolled in the IEE computer classrooms and at home via remote access software.

h. Necessary resources

- Course material will be available in the virtual classroom: class notes, wordings and solutions of exams/exercises, videos …
- Commercial software. Since this software is licensed by the UVa, students agree to use it exclusively for the activities of the course, not being allowed to use it for other purposes. If you plan to use it in any research activity, you must previously inform the teacher responsible, indicating if there is any company or third party involved.

i. Timing

(see section 4.e)

5. Teaching methods

Classes are developed in the computer room in a practical way. The professor guides the class by explanations followed by the development of practical cases. Examples are provided to students to build on the knowledge acquired in the classes.

6. Table of student dedication to the subject

ON-SITE AND PRESENTIAL ON-LINE ACTIVITIES (1)	HOURS	OFF-SITE ACTIVITIES	HOURS
Computing room classes	35	Self-study and individual work	40
Practical classes	5	Study and autonomous group work	28
Workshops	5		
Total presencial	**45**	Total no presencial	**68**
		TOTAL presencial + no presencial	**113**

(1) Presential on-line activity is when a group follows a videoconference synchronously to the class given by the teacher for another group present in the classroom.

7. Assessment methods – Summary table

ACTIVITY	WEIGHT ON FINAL MARK	COMMENTS
Written exam	35%	
Assignments	60%	3 Assignments
Participation in the activities developed in the classroom	5%	

ASSESSMENT CRITERIA

• **Ordinary exam:**
  ○ A minimum mark of 4.0 is required in the written exam to pass.
  ○ A minimum global mark of 5.0 is required to pass.
• **Extraordinary exam:**
  ○ The student can choose between two options: 1) the same criteria as in the ordinary exam, or 2) Written exam with 100% weight on final mark (minimum mark of 5.0 is required in this case to pass).

8. Closing remarks