Proyecto/Guía docente de la asignatura

Course/ Asignatura	Modelado Termodinámico de Procesos Químicos / Thermodynamic Modelling of Chemical Processes		
Unit / Materia	Thermodynamics and Transport in Chemical Processes / Termodinámica y Transporte en los Procesos Químicos		
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	53740
Period/ Periodo de impartición	1st Semester / 1er 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	ÁNGEL MARTÍN MARTÍNEZ SERGIO BORDEL		
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Department / Departamento	Ingeniería Química y Tecnología del Medio Ambiente [Edificio Dr. Mergelinal]		
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 first semester of the first year of the Master's degree in Chemical Engineering. This is a practical course in which students learn how to pose, code and calculate simulation problems. The thermodynamic modelling of industrial processes and their simulation is studied with a fundamental approach.

1.2 Relationship with other subjects

It is the basis for simulation and design subjects.

1.3 Prerequisites

Basic knowledge of chemical thermodynamics and process thermodynamics, as well as general knowledge - matter and energy balances, flow diagrams - of stationary processes, at Chemical Engineering Degree level.

2. Learning outcomes

2.1 Basic

CG01. Ability to apply the scientific method and the principles of engineering and economics, to formulate and solve complex problems in processes, equipment, installations and services, in which the matter undergo changes in its composition, state or energy content, characteristic of the chemical industry and other related sectors, including the pharmaceutical, biotechnological, materials, energy, food or environmental sectors.

CG05. 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.

CG11. Knowing how to establish mathematical models and develop them through the appropriate computer science, as a scientific and technological basis for the design of new products, processes, systems and services, and for the optimization of others already developed.

2.2 Specific

3. Aims

Represent in detail the behavior of processes involving different phases with a very non-ideal behavior and/or unusual conditions, using thermodynamic models adequate. Acquire criteria and use tools for evaluating the reliability and consistency of the results.

Model the behavior of simple and complex reaction processes.

Develop mathematical models and fundamental programmatic tools for calculating processes associated with them in the fields of conditions, including states of aggregation, and energy flows. Use these tools for the purpose of exploring operating conditions and optimization of processes.

4. Contents

Workload in ECTS credits: 4.5

a. Contextualization and justification

(see section 1.1)

b. Learning objectives

Represent in detail the behavior of processes that involve different phases with a very non-ideal behavior and/or unusual conditions.

Acquire criteria and use tools for the evaluation of the reliability and consistency of the results

Model the behavior of complex reaction processes. Acquire the fundamentals of process and device design guided by optimization methods.

c. Syllabus

- Activity coefficient models
- Equations of State, alpha functions, mixing rules
- Calculation of properties with activity coefficient models and equations of state
- Isentropic, isenthalpic processes
- Phase Equilibrium: Advanced Correlation Methods, Phase Space, High Pressure, Electrolytes
- Resolution of phases in multi-component systems
- Chemical reaction equilibrium

d. Teaching methods

Brief exposition of the fundamental theoretical principles complemented with bibliographical material. Development in the classroom, in a cooperative and guided way, of open-ended problems that address the design and simulation of chemical processes or integrating operations. Said development will include a strong component of calculation and analysis of results. Works of different complexity will be proposed for their resolution by the students, which will form the component with the greatest load of the subject.

e. Workplan

Weeks 1 – 15 Development of theoretical foundations and tools, with an assignment every two weeks, to propose and begin to solve in the classroom

f. Assessment

(see section 7)

g Training material

g.1 Basic Bibliography

g.2 Additional Bibliography

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

h. Necessary resources

- Course material will be available in the virtual classroom: class notes, wordings and solutions of exams/exercises …
- Programming software: MatLab, Gnu/Octave, Python

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, and begin to solve in the classroom.

6. Table of student dedication to the subject

ON-SITE AND PRESENTIAL ON-LINE ACTIVITIES (1)	HOURS	OFF-SITE ACTIVITIES	HOURS
Computing room classes	10	Self-study and individual work	67
Practical classes	10		
Workshops	25		
Total presencial	**45**	Total no presencial	**67**
		TOTAL presencial + no presencial	**112**

7. Assessment methods – Summary table

ACTIVITY	WEIGHT ON FINAL MARK	COMMENTS
Written exam	35%	
Assignments	60%	4-6 Assignments. Oral presentation of the assignments may be required.
Participation in the activities developed in the classroom	5%	

ASSESSMENT CRITERIA

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

8. Closing remarks