Proyecto/Guía docente de la asignatura
Project/Course Syllabus

Asignatura ***Course***	Modelado Termodinámico de Procesos Químicos / Thermodynamic Modelling of Chemical Processes		
Materia ***Subject area***	Thermodynamics and Transport in Chemical Processes / Termodinámica y Transporte en los Procesos Químicos		
Módulo ***Module***	Process & Product Engineering / Ingeniería de Procesos y Producto		
Titulación ***Degree Programme***	Master in Chemical Engineering/ Máster en Ingeniería Química		
Plan ***Curriculum***	542	**Código** **Code**	53740
Periodo de impartición ***Teaching Period***	1st Semester / 1er CUATRIMESTRE	**Tipo/Carácter** ***Type***	COMPULSORY / OBLIGATORIA
Nivel/Ciclo ***Level/Cycle***	Master	**Curso** ***Course***	1º
Créditos ECTS ***ECTS credits***	4.5 ECTS		
Lengua en que se imparte ***Language of instruction***	English		
Profesor/es responsable/s ***Responsible Teacher/s***	SERGIO BORDEL VELASCO		
Datos de contacto (E-mail, teléfono…) ***Contact details (e-mail, telephone…)***	sergio.bordel@uva.es		
Departamento ***Department***	Ingeniería Química y Tecnología del Medio Ambiente		
Fecha de revisión por el Comité de Título ***Review date by the Degree Committee***	13/07/2026		

En caso de guías bilingües con discrepancias, la validez será para la versión en español.
In the case of bilingual guides with discrepancies, the Spanish version will prevail.

1. Situación / Sentido de la Asignatura

Course Context and Relevance

1.1 Contextualización

Course Context

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 Relación con otras materias

Connection with other subjects

This subject belongs to the module "Process and Product Engineering", and is considered closely related to other subjects of the module in the same semester, especially with 53747 DISEÑO DE PROCESOS CON REACCIÓN, 53748 DISEÑO DE PROCESOS DE TRANSFERENCIA DE MATERIA and 53749 ANALISIS DE PROCESOS QUIMICOS CON SIMULADORES

1.3 Prerrequisitos

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. Resultados del proceso de formación y de aprendizaje (RD 822/2021) o competencias (RD 1393/2007)

Learning outcomes (RD 822/2021) or competences (RD 1393/2007)

2.1 (RD1393/2007) Competencias Generales

General Competences

CG01. Capacidad para aplicar el método científico y los principios de la ingeniería y economía, para formular y resolver problemas complejos en procesos, equipos, instalaciones y servicios, en los que la materia experimente cambios en su composición, estado o contenido energético, característicos de la industria química y de otros sectores relacionados entre los que se encuentran el farmacéutico, biotecnológico, materiales, energético, alimentario o medioambiental.

CG05. Saber establecer modelos matemáticos y desarrollarlos mediante la informática apropiada, como base científica y tecnológica para el diseño de nuevos productos, procesos, sistemas y servicios, y para la optimización de otros ya desarrollados.

CG11. Poseer las habilidades del aprendizaje autónomo para mantener y mejorar las competencias propias de la ingeniería química que permitan el desarrollo continuo de la profesión

2.2 (RD1393/2007) Competencias Específicas

Specific Competences

CEP01. Aplicar conocimientos de matemáticas, física, química, biología y otras ciencias naturales, obtenidos mediante estudio, experiencia, y práctica, con razonamiento crítico para establecer soluciones viables económicamente a problemas técnicos.

CEP03. Conceptualizar modelos de ingeniería, aplicar métodos innovadores en la resolución de problemas y aplicaciones informáticas adecuadas, para el diseño, simulación, optimización y control de procesos y sistemas.

3. Objetivos

Course Objectives

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. Contenidos y/o bloques temáticos
Course Contents and/or Modules

Bloque 1: Thermodynamic modelling of chemical processes

Carga de trabajo en créditos ECTS: 4,5
Workload in ECTS credits:

a. Contextualización y justificación
a. Context and rationale

Thermodynamic methods to model physical properties and chemical processes are taught in a practical way, including calculation examples with scientific computing software.

b. Objetivos de aprendizaje
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. Contenidos
c. Contents

- 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. Métodos docentes
d. Teaching and Learning methods

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. Plan de trabajo

e. Work plan

Development of theoretical foundations and tools, with computing assignments, to propose and begin to solve in the classroom

f. Evaluación

f. Assessment

See section 7

g Material docente

g Teaching material

g.1 Bibliografía básica

Required Reading

A.R.H. Goodwin, J. V. Sengers, C. J. Peters. Applied Thermodynamics of Fluids. RSC Publishing, 2010

J M Prausnitz, R. N. Lichtenthaler, E. G. de Azevedo. Molecular Thermodynamics of fluid-phase equilibria, 2nd ed. Prentice Hall, 1985.

g.2 Bibliografía complementaria

Supplementary Reading

g.3 Otros recursos telemáticos (píldoras de conocimiento, blogs, videos, revistas digitales, cursos masivos (MOOC), …)

Additional Online Resources (microlearning units, blogs, videos, digital journals, massive online courses (MOOC), etc.)

h. Recursos necesarios

Required 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. Temporalización

Course Schedule

CARGA ECTS *ECTS LOAD*	**PERIODO PREVISTO DE DESARROLLO** *PLANNED TEACHING PERIOD*
4,5 ECTS	Weeks 1-15

5. Métodos docentes y principios metodológicos

Instructional Methods and guiding methodological principles

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. Tabla de dedicación del estudiantado a la asignatura

Student Workload Table

ACTIVIDADES PRESENCIALES o PRESENCIALES o A DISTANCIA[(1)] *FACE-TO-FACE/ ON-SITE or ONLINE ACTIVITIES [(1)]*	**HORAS** HOURS	**ACTIVIDADES NO PRESENCIALES** *INDEPENDENT / OFF-CAMPUS WORK*	**HORAS** HOURS
Theory classes	25	Self-study	67,5
Practical classes	10		
Computing seminars	10		
Total presencial *Total face-to-face*	**45**	Total no presencial. *Total non-face-to-face*	**67,5**
		TOTAL presencial + no presencial *Total*	**112,5**

(1) Actividad presencial a distancia es cuando un grupo sentado en un aula del campus sigue una clase por videoconferencia de forma síncrona, impartida por el profesor. *Distance face-to-face activity refers to a situation in which a group of students, seated in a classroom on campus, attends a class via live videoconference delivered by the instructor in real time.*

7. Sistema y características de la evaluación

Assessment system and criteria

INSTRUMENTO/PROCEDIMIENTO *ASSESSMENT METHOD/PROCEDURE*	**PESO EN LA NOTA FINAL** *WEIGHT IN FINAL GRADE*	**OBSERVACIONES** REMARKS
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%	

CRITERIOS DE CALIFICACIÓN *ASSESSMENT CRITERIA*
• **Convocatoria ordinaria. First Exam Session (Ordinary)** ○ Written exam + assignments. A minimum global mark of 5.0 is required to pass.

- **Convocatoria extraordinaria(*)Second Exam Session (Extraordinary / Resit) (*):**
  - 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
- **Convocatoria extraordinaria de fin de carrera(*) Extraordinary exam for end of degree:**
  - El alumnado que se acoja a la convocatoria extraordinaria de fin de carrera será evaluado mediante una prueba global que permita acreditar la adquisición de las competencias y resultados. Incluyendo examen teórico y tarea de cálculo para realizar en clase.

8. Consideraciones finales

Final remarks

The use of artificial intelligence (AI) tools as support in the development of assignments, reports, and other assessable documents is authorized, provided that such use is clearly specified in each submission. Students must explicitly indicate which AI tools were used, as well as the type of assistance provided (for example, text generation, data analysis, programming, etc.), in order to ensure transparency and promote the ethical use of these technologies.