Proyecto docente de la asignatura

Course/ Asignatura	Chemical Process Analysis with Simulators / Análisis de Procesos Químicos con Simuladores		
Unit / Materia	Process & Product Engineering / Ingeniería de Procesos y Producto		
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	JUAN GARCÍA SERNA RAFAEL B. MATO CHAÍN		
Contact / Datos de contacto (E-mail, teléfono…)	jgserna@iq.uva.es, 983 184 934 rbmato@iq.uva.es, 983 423 177		
Tutoring Schedule / Horario de tutorías	Monday, Tuesday and Wednesday from 12:00 to 14:00. It is recommended to make an appointment. / Lunes, Martes y Miércoles de 12:00 a 14:00. Recomendable concertar cita.		
Department / Departamento	Ingeniería Química y Tecnología del Medio Ambiente [Edificio Residencia Alfonso VIII]		

1. Location / Sense of the Subject

1.1 Contextualization

This course is taught in the second semester of the first year of the Master in Chemical Engineering. It is a subject of marked practical character where students learn the use of commercial simulation software of chemical processes. It is deepened in the thermodynamic modelling of industrial processes and in their dynamic simulation.

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.
- Learn how to transform steady state simulations into dynamic ones, using HYSYS.
- Use dynamic simulations to analyse and optimize process operation.
- Learn to select, evaluate, tune up and optimize the thermodynamic modelling of component mixtures under specific operation conditions.

4. Contents

Workload in ECTS credits: 3.0

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 4: Assignment 1
Week 4: Start of Dynamic section
Week 9: Assignment 2
Week 10: Start of Properties section
Week 14: Assignment 3

f. Assessment

(see section 7)

g. Basic resources

- Guías de usuario del software HYSYS (AspenTech).
- Guías de usuario del software Aspen Properties (AspenTech).

h. Complementary resources

i. Necessary resources

HYSYS and Aspen Properties software

j. 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 classroom.

7. Study hours

ON-SITE ACTIVITIES	HOURS	OFF-SITE ACTIVITIES	HOURS
Lectures	15	Self-study and individual work	40
Practical classes	5	Study and autonomous group work	28
Workshops	5		

Computing room classes	20		
Total on-site	**45**	**Total off-site**	**68**

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:** o A minimum mark of 4.0 is required in the written exam to pass. • **Extraordinary exam:** o A minimum mark of 4.0 is required in the written exam to pass. o Assignments marks (60%) and class activity (5%) marks are preserved to calculate the final value.

8. Closing remarks