

**Proyecto/Guía docente de la asignatura Adaptada a la Nueva Normalidad**

Se debe indicar de forma fiel cómo va a ser desarrollada la docencia. Esta guía debe ser elaborada teniendo en cuenta a todos los profesores de la asignatura. Conocidos los espacios y profesorado disponible, se debe buscar la máxima presencialidad posible del estudiante siempre respetando las capacidades de los espacios asignados por el centro y justificando cualquier adaptación que se realice respecto a la memoria de verificación. Si la docencia de alguna asignatura fuese en parte online, deben respetarse los horarios tanto de clase como de tutorías). La planificación académica podrá sufrir modificaciones de acuerdo con la actualización de las condiciones sanitarias.

<b>Course/ Asignatura</b>	Chemical Process Analysis with Simulators / Análisis de Procesos Químicos con Simuladores		
<b>Unit / Materia</b>	Process & Product Engineering / Ingeniería de Procesos y Producto		
<b>Module / Módulo</b>	Process & Product Engineering / Ingeniería de Procesos y Producto		
<b>Degree / Titulación</b>	Master in Chemical Engineering/ Máster en Ingeniería Química		
<b>Plan Code / Plan</b>	542	<b>Couse code/ Código</b>	53749
<b>Period/ Periodo de impartición</b>	2nd Semester / 2º CUATRIMESTRE	<b>Type / Tipo/Carácter</b>	COMPULSORY / OBLIGATORIA
<b>Level/Cycle / Nivel/Ciclo</b>	MÁSTER	<b>Year / Curso</b>	1º
<b>ECTS credits / Créditos ECTS</b>	4.5 ECTS		
<b>Language / Lengua en que se imparte</b>	ENGLISH / INGLÉS		
<b>Staff / Profesor/es responsable/s</b>	ÁNGEL MARTÍN MARTÍNEZ RAFAEL B. MATO CHAÍN		
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<b>Department / Departamento</b>	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. This is a highly practical course in which students learn the use of 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.
- 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

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(see section 5)

#### e. Workplan

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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

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(see section 7)

#### g Training material

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##### g.1 Basic Bibliography

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- HYSYS Software User Guides (AspenTech).
- Aspen Properties Software User Guides (AspenTech).

##### g.2 Additional Bibliography

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

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The course Web page on Campus Virtual includes links to the videos with the theoretical contents of the subject.

#### h. Necessary resources

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- Course material will be available in the virtual classroom: class notes, wordings and solutions of exams/exercises, videos ...
- Computer classroom with commercial software
- As this software is licensed by UVa, students are committed to using it exclusively for the course activities, not being allowed its use for other purposes. If you plan to use it in any research activity, you must inform the teacher in charge in advance, indicating whether there is a company or third party involved.

#### i. Timing

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(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.

## 6. Table of student dedication to the subject

ON-SITE AND PRESENTIAL ON-LINE ACTIVITIES <sup>(1)</sup>	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 presencial	<b>45</b>	Total no presencial	<b>68</b>
TOTAL presencial + no presencial			<b>113</b>

(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.
- **Extraordinary exam:**
  - A minimum mark of 4.0 is required in the written exam to pass.
  - The exam will be carried out in a similar way to the ordinary call in both blocks. Only the final weight of each contribution to the final mark will be modified:
    - Oral exam: 65%
    - Assignments: 35%

## 8. Closing remarks