UNIVERSIDAD DE CASTILLA - LA MANCHA
GUÍA DOCENTE

1. General information

Course:	SIMULATION OF CHEMICAL AND ENERGY PREOCESSES	**Code:**	57744
Type:	ELECTIVE	**ECTS credits:**	6
Degree:	344 - CHEMICAL ENGINEERING	**Academic year:**	2022-23
Center:	1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY	**Group(s):**	21
Year:	4	**Duration:**	First semester
Main language:	Spanish	**Second language:**	English
Use of additional languages:		**English Friendly:**	Y
Web site:		**Bilingual:**	N

Lecturer: **JESUS MANUEL GARCIA VARGAS** - Group(s): **21**

Building/Office	**Department**	**Phone number**	**Email**	**Office hours**
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Lecturer: **JOSE LUIS VALVERDE PALOMINO** - Group(s): **21**

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2. Pre-Requisites

Not established

3. Justification in the curriculum, relation to other subjects and to the profession

Justification in the curriculum and relationship with the profession

This subject allows to complete the training within the degree in Chemical Engineering in process simulation initiated in previous courses in subjects like METHODS AND COMPUTER APPLICATIONS IN CHEMICAL ENGINEERING, FLUID MECHANICS, HEAT TRANSMISSION, THERMOTECHNICS and INTEGRATED LABORATORY OF BASIC OPERATIONS AND ENGINEERING OF THE CHEMICAL REACTION, and will serve as a tool for others such as CARBON, OIL AND PETROLEOCHEMICAL TECHNOLOGY, PROJECTS and FINAL DEGREE WORK and other subject of the MASTER'S DEGREE IN CHEMICAL ENGINEERING. Undoubtedly the knowledge of the simulation of processes can be used profusely by future graduates to study the stationary and dynamic behavior of industrial chemical processes.

The main goal of this subject is that the students obtain a high skill in the use of the two main simulators of processes in stationary state: ASPEN HYSYS and ASPENPLUS. This training will be of great help for the course PROCESS DINAMICS. CONTROL OF INDUSTRIAL PLANTS that is taught in the aforementioned Master.

To this end, the subject is organized through the case method in order that students discover the peculiarities of the different modules used in the simulation of complex chemical processes and real plants.

4. Degree competences achieved in this course

Course competences

Code	Description
E26	Knowledge and capacity of management and specification of the main industrial equipment in the area of knowledge of chemical engineering
E44	Ability to write, sign and develop projects in the field of chemical engineering that are intended, according to the knowledge acquired as established in section 5 of order CIN / 351/2009 of February 9, construction, reform, repair, conservation, demolition, manufacture, installation, assembly or operation of: structures, mechanical equipment, energy installations, electrical and electronic installations, industrial facilities and processes and manufacturing and automation processes.
G01	Capacity for the direction, of the activities object of the engineering projects described in the competence G1.
G03	Ability to solve problems with initiative, decision making, creativity, critical reasoning and to communicate and transmit knowledge, skills and abilities in the field of Chemical Engineering.
G10	Knowledge, understanding and ability to apply the necessary legislation in the exercise of the profession of Industrial Technical Engineer
G12	Knowledge of Information and Communication Technologies (ICT).
G13	Proper oral and written communication
G14	ethical commitment and professional ethics
G16	Capacity for critical thinking and decision making
G17	Synthesis capacity
G18	Capacity for teamwork
G19	Ability to analyze and solve problems
G20	Ability to learn and work autonomously
G21	Ability to apply theoretical knowledge to practice
G22	Creativity and initiative
G23	Leadership

5. Objectives or Learning Outcomes

Course learning outcomes

Description

To be able to use the ASPEN simulator in the simulation of basic operations of fluids, heat and transfer of matter and in the calculation of reactors.

Be able to simulate known chemical and energetic processes with the two simulators listed above and comparison of results.

To be able to handle the basic concepts of conceptual design, optimization and calculations of energy conservation and thermodynamic efficiency of chemical processes.

Be able to improve your simulation capabilities with HYSYS tools.

6. Units / Contents

Unit 1: Basic concepts of simulation. Introduction. Degree of freedom. Equilibrium conditions. Equilibrium relationships between phases. Equilibrium between phases based on equations of state and activity coefficients. Hypothetical components. Phase and enthalpic diagrams. Examples.

Unit 2: Simulation of separation operations. Simulation of flash distillation, rectification and absorption. Approximate and rigorous calculation methods. Simulation of liquid-liquid extraction in one and several equilibrium stages. Examples.

Unit 3: Logical unit operations and sizing of separation equipment. Logical unit operations in HYSYS: ADJUST, RECYCLE and SET. Staged columns and packed columns. Sizing. Examples.

Unit 4: Simulation of chemical reactors. Introduction. Equilibrium reactor. Continuous stirred-tank reactor. Plug flow reactor. Examples.

Unit 5: Introduction to the use of ASPEN. Overview. Practical case of use of the ASPEN PLUS simulator. Examples.

Unit 6: Simulation of unitary operations. Introduction. Mixers and splitters. Fluid impellers. Valves and pipes. Heat exchange equipment. Separation and flash distillation. Decanters. Distillation, liquid-liquid extraction and absorption. Examples.

Unit 7: Advanced simulation of separation operations. The RadFrac module. Convergence with the RadFrac module. Examples.

Unit 8: Simulation of chemical reactors. Introduction. Types of chemical reactions. Kinetics of chemical reactions. Types of chemical reactors. Continuous stirred-tank reactor. Continuous plug flow reactor. Discontinuous stirred-tank reactor. Examples.

Unit 9: Conceptual analysis of chemical processes. Introduction. Flowsheet analysis. Equilibrium of binary mixtures. Residue curves. Sensitivity analysis. Design specifications. Convergence. Examples.

Unit 10: Simulation of chemical processes with Aspen HYSYS and ASPEN PLUS. Simulation and analysis of chemical plants. Comparison of results. Examples.

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Computer room practice [ON-SITE]	Practical or hands-on activities	E26 E44 G01 G03 G10 G12 G13 G16 G17 G18 G20 G21 G22 G23	2.1	52.5	N	-	
Study and Exam Preparation [OFF-SITE]	Self-study	E26 E44 G01 G03 G10 G12 G13 G16 G17 G18 G19 G20 G21 G22 G23	3.6	90	Y	N	
Final test [ON-SITE]	Assessment tests	E26 E44 G01 G03 G10 G12 G13 G16 G17 G18 G20 G21 G22 G23	0.1	2.5	Y	Y	
Group tutoring sessions [ON-SITE]	Project/Problem Based Learning (PBL)	E26 E44 G01 G03 G10 G12 G13 G16 G17 G18 G19 G20 G21 G22 G23	0.1	2.5	N	-	
Workshops or seminars [ON-SITE]	Project/Problem Based Learning (PBL)	E26 E44 G01 G03 G10 G12 G13 G16 G17 G18 G20 G21 G22 G23	0.1	2.5	Y	N	
		Total:	**6**	**150**			
		Total credits of in-class work: 2.4					**Total class time hours: 60**
		Total credits of out of class work: 3.6					**Total hours of out of class work: 90**

As: Assessable training activity

Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Final test	40.00%	40.00%	
Assessment of problem solving and/or case studies	40.00%	40.00%	
Projects	20.00%	20.00%	
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

The evaluation of this course will require the completion of a series of activities to which the percentage weight previously indicated corresponds:

1. An exam with practical questions on the contents taught in the course.
2. Resolution of various simulation problems.
3. Resolution of a practical case solved in group and defended publicly.

The course will be passed provided that in each of these evaluation activities a minimum mark of 4.0/10 is reached and an average value for all of them higher than 5.0/10.

Non-continuous evaluation:

In the final test, additional activities will be proposed to evaluate the competences referred to Problem Solving or Cases and the student will also have to present that day a work similar to the one proposed for the group.

Specifications for the resit/retake exam:

he evaluation of this course will require the completion of a series of activities to which the percentage weight previously indicated corresponds:

1. An exam with practical questions on the contents taught in the course.
2. Resolution of different simulation problems.
3. Resolution of a case study defended publicly.

The course will be passed provided that in each of these evaluation activities a minimum mark of 4.0/10 is achieved and an average value for all of them higher than 5.0/10.

9. Assignments, course calendar and important dates

Not related to the syllabus/contents	
Hours	**hours**
Computer room practice [PRESENCIAL][Practical or hands-on activities]	52.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	90
Final test [PRESENCIAL][Assessment tests]	2.5
Group tutoring sessions [PRESENCIAL][Project/Problem Based Learning (PBL)]	2.5
Workshops or seminars [PRESENCIAL][Project/Problem Based Learning (PBL)]	2.5

Unit 1 (de 10): Basic concepts of simulation. Introduction. Degree of freedom. Equilibrium conditions. Equilibrium relationships between phases. Equilibrium between phases based on equations of state and activity coefficients. Hypothetical components. Phase and enthalpic diagrams. Examples.

Comment: The calendar is approximate as it will depend on the beginning of the school year and holidays. This should be corrected administratively. They are taught one hour each day during the weeks of the course with the design approved by the Faculty Board.

Global activity	
Activities	**hours**
Group tutoring sessions [PRESENCIAL][Project/Problem Based Learning (PBL)]	2.5
Computer room practice [PRESENCIAL][Practical or hands-on activities]	52.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	90
Workshops or seminars [PRESENCIAL][Project/Problem Based Learning (PBL)]	2.5
Final test [PRESENCIAL][Assessment tests]	2.5
Total horas:	150

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Biegler, L. T.	Systematic methods of chemical process design	Prentice Hall		0-13-492422-3	1997	
Douglas, James M.	Conceptual design of chemical processes	McGraw-Hill		0-07-017762-7	1988	
Luyben, William L.	Distillation design and control using AspenTM simulation	John Wiley & Sons		0-471-77888-5	2006	
Luyben, William L.	Plantwide dynamic simulators in chemical processing and cont	Marcel Dekker		0-8247-0801-6	2002	
Luyben, William L.	Process modeling, simulation, and control for chemical engin	McGraw-Hill		0-07-039159-9	1990	
Shinskey, F. G.	Sistemas de control de procesos : aplicación, diseño y sinto	McGraw-Hill		970-10-0934-7	1996	