UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course:	SIMULATION OF CHEMICAL AND ENVIRONMENTAL PROCESSES	**Code:**	57746
Type:	ELECTIVE	**ECTS credits:**	6
Degree:	344 - CHEMICAL ENGINEERING	**Academic year:**	2023-24
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: **ANA MARIA BORREGUERO SIMON** - Group(s): **21**

Building/Office	**Department**	**Phone number**	**Email**	**Office hours**
Enrique Costa Novella/Despacho 12	INGENIERÍA QUÍMICA	6353	anamaria.borreguero@uclm.es	Wednesday, Thursday and Friday from 10 to 11. Preferably make an appointment via email.

Lecturer: **MARIA LUZ SANCHEZ SILVA** - Group(s): **21**

Building/Office	**Department**	**Phone number**	**Email**	**Office hours**
Enrique Costa. Despacho 12	INGENIERÍA QUÍMICA	6307	marialuz.sanchez@uclm.es	Monday, Tuesday and Friday from 9:30 to 11:30. Preferably make an appointment via email.

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 about integration of processes and operations
E44	Capacity to handle process simulators in Chemical Engineering
G01	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.
G03	Knowledge in basic and technological subjects, which enables them to learn new methods and theories, and give them versatility to adapt to new situations.
G10	Ability to work in a multilingual and multidisciplinary environment.
G12	Proficiency in a second foreign language at level B1 of the Common European Framework of Reference for Languages
G13	Knowledge of Information and Communication Technologies (ICT).
G14	Proper oral and written communication
G16	Management capacity and information planning
G17	Capacity for critical thinking and decision making
G18	Synthesis capacity
G19	Capacity for teamwork
G20	Ability to analyze and solve problems
G21	Ability to learn and work autonomously
G22	Ability to apply theoretical knowledge to practice
G23	Creativity and initiative

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Be able to use the Aspen simulator in the simulation of basic fluid operations, heat and material transfer and in the calculation of reactors.

Be able to improve your simulation capabilities with HYSYS tools.

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

Be able to manage the basic concepts for the analysis, conceptual design, optimization and treatment of gaseous and liquid effluents, to account for the equivalent CO2 emissions generated by chemical processes, and to acquire data from simulators necessary to establish the life cycle analysis and the environmental impact of the same.

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 Aspen 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 Plus. 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 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 G19 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 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%	Includes the problems proposed for individual resolution and the problem of a more complex overall process proposed for group solution
Projects	20.00%	20.00%	Corresponds to the presentation and defense of the work presented in group.
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 corresponds the percentage weight previously indicated:

1. An exam with practical questions on the contents taught in the course.

2. Resolution of different simulation problems.
3. Resolution of a practical case solved in group and defended publicly.
Students qualify in case of obtaining a minimum grade of 4.0/10 on each one of these evaluation activities 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:

The evaluation of this course will require the completion of a series of activities to which corresponds the percentage weight previously indicated:
1. An exam with practical questions on the contents taught in the course.
2. Resolution of different simulation problems.
3. Resolution of a practical case solved in group and defended publicly.
Students qualify in case of obtaining a minimum grade of 4.0/10 on each one of these evaluation activities and an average value for all of them higher than 5.0/10.

Specifications for the second resit / retake exam:

No special criteria

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
Group tutoring sessions [PRESENCIAL][Project/Problem Based Learning (PBL)]	2.5

Global activity

Activities	hours
Computer room practice [PRESENCIAL][Practical or hands-on activities]	52.5
Study and Exam Preparation [AUTÓNOMA][Self-study]	90
Group tutoring sessions [PRESENCIAL][Project/Problem Based Learning (PBL)]	2.5
Total horas:	145

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	
Luyben, William L.	Distillation design and control using AspenTM simulation	John Wiley & Sons		0-471-77888-5	2006	
Shinskey, F. G.	Sistemas de control de procesos : aplicación, diseño y sinto	McGraw-Hill		970-10-0934-7	1996	
Douglas, James M.	Conceptual design of chemical processes	McGraw-Hill		0-07-017762-7	1988	
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	