PERSONA CIÈNCIA EMPRESA
UNIVERSITAT RAMON LLULL

COURSE: PROCESS SIMULATION

SUBJECT MATTER: Simulation and Process Control
MODULE: Specific Technology
PROGRAM: Degree in Chemical Engineering

GENERAL CHARACTERISTICS

Type: ☐ Basic Formation, ☑ Compulsory, ☐ Elective
☐ Final Degree Project, ☐ Internship

Duration: Semestral **Semester/s**: 7
Number of ECTS credits: 5
Language/s: Spanish

DESCRIPTION

SHORT DESCRIPTION AND JUSTIFICATION

The use of process simulation tools -from spreadsheets to specific software packages- is something that is part of the day-to-day of an engineer in any task related to the synthesis, design, improvement and, even, operation of industrial processes.

It should be noted that it is not an objective of this course to be a step in the Numerical Analysis training of the future Engineer, neither to be an extension of algorithmic and computer programming. In it, the use of computers is seen as something natural, currently essential in tasks of calculation, and the software packages used, as a mere example of how much is on the market today.

This course takes place mainly in case studies on practical examples and, as far as possible, real cases.

COMPETENCES

- Be able to understand and apply knowledge of Chemistry and Engineering for application in the field of Chemical Engineering. (CB1, E2)
- Be able to use systems, components or processes to achieve the requirements established in the activity to be carried out in the field of Chemical Engineering. (CB2, E6)
- Be able to identify, formulate and solve problems in the fields of Chemical Engineering and Chemistry. (CB2, E7)
- Be able to analyze, integrate and interpret data and information from the field of Chemical Engineering. (CB3, E8)
- Ability to analyze, design, simulate and optimize processes and products. (TE2)
- Ability to design, manage and operate chemical process instrumentation, simulation and control. (TE4)

PREREQUISITES

According to current academic teaching planning and regulations.

CONTENTS

1. **Material and energy balances in steady state**
   Example to be developed: Balance of plant

2. **Application of graphs to solving systems of equations**
   Example to be developed: Boolean operations with Matlab

3. **Simulation from ordinary differential equations**
   Example to be developed: Batch Reactor

4. **Simulation from partial differential equations**
   Example to be developed: Tubular Reactor

5. **Sensitivity, objective function and nonlinear regression**
   Example to be developed: Batch Reactor

6. **Simulation of chemical processes with HYSYS™**
   Example to be developed: Unit operations of chemical process

METHODOLOGY

LEARNING ACTIVITIES

Learning activities	Hours	ECTS Credits	Competences
Lectures	32	1.2	CB1, E2, CB2, E6, TE2, TE4
Case and Problem-Solving Sessions	5	0.2	CB2, E7, CB3, E8, TE2, TE4
Seminars		0	
Practical & Lab Work	24	1.0	CB2, E7, CB3, E8, TE2, TE4
Presentations		0	
Personal study	64	2.2	CB1, E2, CB2, E6, E7, CB3, E8, TE2, TE4
Assessment Tasks (Exams, Continuous Assessment...)	10	0.4	CB1, E2, CB2, E6, E7, CB3, E8, TE2, TE4
TOTAL	**135**	**5.0**	

TEACHING METHODOLOGY

The teaching methods used in the course uses an explanatory dynamic (presentation of content) where the different theoretical concepts are presented.

Students have one hour weekly of laboratory where they practice using the basic software tools of the course with their own computer. To do this, they receive a presentation-tutor, who guide them in the development of practices. Also, they develop a simulation project of an industrial process in teams of four people along the course.

For the student's personal study, the necessary software, problems proposed for individual work, relevant documents to assist in the practical sessions and library resources are provided.

Is necessary to have a laptop for this course.

ASSESSMENT

ASSESSMENT METHODS

Assessment Methods	Weight	Competences
Final Exam	40%	CB1, E2, CB2, E6, E7, CB3, E8, TE2, TE4
Continuous Assessment Activities	10%	CB2, E7, CB3, E8, TE2, TE4
Lab or Field Work	10%	CB2, E7, CB3, E8, TE2, TE4
Projects	40%	CB1, E2, CB2, E6, E7, CB3, E8, TE2, TE4

LEARNING OUTCOMES

- The student must demonstrate the assimilation of basic information provided in the course, being able to express it in a clear and concise language. (CB1, E2, CB2, E6, E7, CB3, E8, TE2, TE4).
- The student must demonstrate proficiency in formulating problems and, where appropriate, in its solution with limited resources. (CB1, E2, CB2, E6, E7, CB3, E8, TE2, TE4).
- The student must show ability to select the most appropriate simulation tools to solve each problem. (CB1, E2, CB2, E6, E7, CB3, E8, TE2, TE4).

QUALIFICATION

The evaluation of the course will consider the marks obtained in the laboratory, in the simulation project and the final exam.

It is a necessary condition to pass the course have passed the laboratory and the simulation project, and the final exam grade exceeds 4.5 points, in addition to schooling in all activities of the course.

In this case the final score is calculated by the following expression in all calls of the subject: 10% Laboratory +10% Continuous Assessment Activities + 40% Simulation Project + 40% Final Exam. Otherwise the final rating is the lower of the ratings of laboratory, simulation project or examination.

If a student fails laboratory or simulation project should apply for recovery. To that qualifications that have been failed can be taken into account in subsequent calls must be delivered in person

one week before the examination of the corresponding call. Otherwise, if the student took the exam, the final grade for the course will be not presented.

ASSESSMENT OF THE COMPETENCES

For the evaluation of CB1/E2 competence it will be used as an indicator the qualification of the theory of final exam and the simulation project. For assessing CB2/E6 competence, it will be used as an indicator the qualification of simulation project. For the assessment of CB2/E7 competence, it is used as an indicator the laboratory, the simulation project and the practical part of the final exam. For the assessment of CB3/E8, TE2 and TE4 competences, the indicator used is the final course grade.

BIBLIOGRAPHY

NUMERICAL METHODS:

- Press, W.H., Teukolsky, S.A., Vetterling, W.T. y Flannery, B.P.; Numerical Recipes 3rd Edition. The Art of Scientific Computing; (Septiembre 2007); Cambridge University Press; Cambridge (ISBN: 0521880688).
- Chapra, Steven C. y Canale, Raymond P.; Numerical Methods for Engineers; 6th Edition, McGraw-Hill Science/Engineering/Math (ISBN 978-0-07-340106-5) http://highered.mcgraw-hill.com/sites/0073401064/information_center_view0/
- Chapra, Steven C. y Canale, Raymond P.; Métodos numéricos para ingenieros; 6a Edición, McGraw-Hill (ISBN 978-607-15-0499-9)

PROPERTIES ESTIMATION:

- Reid, R.C., Prausnitz, J.M. y Poling, B.E.; The Properties of Gases and Liquids; 4th edition (Abril 1987); McGraw Hill Text (ISBN: 0070517991).
- Poling, B.E., Prausnitz, J.M. y O'Connell, J.P.; The Properties of Gases and Liquids; 5th edition (November 2000); McGraw Hill Professional (ISBN: 0070116822).

SIMULATION:

- Himmelblau, D.M. y Bischoff, K.B.; Análisis y Simulación de Procesos; Reverté, Barcelona 1992 (ISBN 84-291-7235-1)
- Cha, P.D., Rosenberg, J.J. y Dym, C.L.; Fundamentals of Modeling and Analyzing Engineering Systems; Cambridge University Press, Cambridge (UK) 2000 (ISBN 0-521-59463-4)

- Seider, W.D., Seader, J.D. y Lewin, D.R.; Process Design Principles: Synthesis, Analysis and Evaluation; John Wiley & Sons, Inc., New York (USA) 1999 (ISBN 0-471-24312-4)
- Seider, W.D., Seader, J.D. y Lewin, D.R.; Product and Process Design Principles: Synthesis, Analysis and Evaluation; 2a edición, (Julio 2003); John Wiley & Sons, Inc., New York (USA) (ISBN 0-471-21663-1)
- Jiménez Gutiérrez, A.; Diseño de procesos en Ingeniería Química; Reverté, Barcelona 2003 (ISBN 84-291-7277-7)
- Turton, R., Bailie R.C., Whiting W.B., Shaeiwitz J.A., Bhattacharyya, D.; Analysis, Synthesis and Design of Chemical Processes; 4th edition, (July 2012); Prentice Hall International Series in the Physical and Chemical Engineering Sciences; Prentice Hall (ISBN 978-0132618120)

DOCUMENT HISTORY

PREVIOUS REVISIONS
September 12, 2017, Dr. José Javier Molins
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September 30, 2014, Dr. José Javier Molins
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March 3, 2013, Dr. José Javier Molins
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