SUBJECT TEACHING GUIDE

G785 - Simulation and Optimisation of Chemical Processes

Degree in Chemical Engineering

Academic year 2023-2024

1. IDENTIFYING DATA				
Degree	Degree in Chemical Engineering		Type and Year	Compulsory. Year 3
Faculty	School of Industrial Engineering and Telecommunications			
Discipline	Subject Area: Process Design, Management and Operation.Simulation, Dynamics, Control and Instrumentation of Chemical Processes. Analysis, Design and Optimisation of Processes and Products Module: Compusory Training Industrial Chemistry			
Course unit title and code	G785 - Simulation and Optimisation of Chemical Processes			
Number of ECTS credits allocated	6	Term	Semester based (2)	
Web				
Language of instruction	Spanish	English Friendly	Yes	Mode of delivery	Face-to-face

Department	DPTO. DE QUIMICA E INGENIERIA DE PROCESOS Y RECURSOS.
Name of lecturer	BERTA GALAN CORTA
E-mail	berta.galan@unican.es
Office	E.T.S. de Ingenieros Industriales y de Telecomunicación. Planta: - 3. DESPACHO PROFESORES (S3015)
Other lecturers	GEMA RUIZ GUTIERREZ

3.1 LEARNING OUTCOMES
- Develop models for chemical process for steady state and dynamic situations. Ability to differentiate and to apply appropriated mathematical models used to describe chemical processes . Resolve simulation problems and propose possible solutions with available simulation tools. Select appropriated techniques to solve optimization problem. Ability to use tools simulation and optimization for the resolution of mass balances, energy balances, design of processes... Ability to use computer tools for the design, simulation and optimization of operations processes in steady-state and dynamic state.

4. OBJECTIVES

1. The main objective of the course is the knowledge of the techniques and tools of simulation and optimization of chemical processes.
2. Other objetive is the development of good habits in the modeling and subsequent resolution of the problems.
3. Developmento of the ability to recognize and resolve situations which require the use of optimization tools, as well as the ability for the mathematical modelling of them.
 4. The knowledge of general concepts of simulation and optimization of chemical processes as well as theoretical concepts to deal with these problems by means of commercial processes software: Aspen Plus, Aspen Custom Modeler and the GAMS optimization program.

6. COURSE ORGANIZATION

	CONTENTS
1	1. Chemical Process Modelling
2	2. Sequential Modular Simularion. Aspen Plus
3	3. Equation Oriented Simulation. Aspen Custom Modeller.
4	5. Lineal Optimization. GAMS
5	5. Non-Lineal Optimization.GAMS
6	6. Optimization with binary variables

7. ASSESSMENT METHODS AND CRITERIA

Description	Type	Final Eval.	Reassessn	%
Exam about Aspen Custom Modeler and Gams	Laboratory evaluation	No	Yes	42,50
Exam about Aspen Plus and theory exam	Laboratory evaluation	No	Yes	42,50
Excercises uploaded in Moodle	Work	No	No	15,00
TOTAL				100,00

Observations
The student can pass the subject through continuous evaluation or presenting a final exam. The continuous evaluation requires: submit the exercises on the proposed dates in Moodle and pass the exams. For students who does not go to the classes regularly, the exam will take place on the date indicated by UC and will consist on one writting test and three computer exams: Aspen Plus, Aspen Custom Modeler and Gams. Besides, the excercise will be evaluated counting fot 15% of the final mark.

Observations for part-time students
For students on part-time, there is an exam consisting of a written test and an three exams at computer using Aspen Plus , Aspen Custom Modeler and Gams.

8. BIBLIOGRAPHY AND TEACHING MATERIALS

BASIC

PUIGJANER L., OLLERO, P., De PRADA, C., JIMENEZ L. Estrategias de modelado, simulación y optimización de procesos químicos. Editorial Síntesis. 2006.

BIEGLER L.T., GROSSMANN I.E., WESTERBERG A.W., Systematic Methods of Chemical Process Design. Prentice Hall. New Jersey, 1997.

GROSSMANN I.E., Advanced Optimization for Process Systems Engineering. Cambridge University Press. 2021

BIEGLER L.T., Nonlinear programming: concepts, algorithms, and applications to chemical processes. 2010.

CABALLERO, R., GÓMEZ, T., GONZÁLEZ, M., MUÑOZ, M.M., REY, L. y RUIZ, F. Programación Matemática para Economistas. 1997.

EDGAR T. F., HIMMELBLAU DAVID M., LASDON LEON S., "Optimization of Chemical Processes", 2001.

FLOUDAS, C.A.; "Nonlinear and Mixed-Integer Optimization" Oxford University Press. 1995.

PUIGJANER, L., OLLERO, P., DE PRADA, C., JIMENEZ L. "Estrategias de modelado, simulación y optimización de procesos químicos". Sinteis. 2006.

SEIDER W. D., SEADER, LEWIN D.R., "Product and process design principles : synthesis, analysis, and evaluation". Wiley & sons. New York, 2010.

SCHEFFLAN R., Teach yourself the basics of Aspen Plus. Hoboken, N.J. Wiley ; New York, American Institute of Chemical Engineers, cop. 2011.

WESTERBERG, A.W., HUTCHISON H.P., MOTARD R.L., WINTER P., Process Flowsheeting, Cambridge University Press, Gran Bretaña. 1985.