

SUBJECT TEACHING GUIDE

G785 - Simulation and Optimisation of Chemical Processes

Degree in Chemical Engineering

Academic year 2021-2022

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 apply appropriately mathematical models used to describe chemical processes .
- Resolve simulation problems and propose possible solutions with available simulation tools.
- Select appropriate techniques to solve optimization problem.
- Ability to use the tools of simulation and optimization for the resolution of mass balances, design of processes...
- Ability to use computer training 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 objective 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	%
Aspen Custom Modeler, Gams	Laboratory evaluation	No	Yes	45,00
Aspen Plus and Theory exam	Laboratory evaluation	No	Yes	45,00
Case studies	Work	No	No	10,00
TOTAL				100,00

Observations

The student can pass the subject through continuous assessment or presenting a final examination. The continuous evaluation requires: assistance to 100% of classes, submit the exercises on the proposed dates in Moodle and pass the exams. The mark of each exam must 5 out of 10 to pass the course. For students not attendint the subject by continuous evaluation, the exam will take place on the date indicated by the school and will be carry out as one wriiting test and three compueter tests: Aspen Plus, Aspen Custom Modeler and Gams.

Observations for part-time students

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

8. BIBLIOGRAPHY AND TEACHING MATERIALS

BASIC

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.