Course guide
820532 - SOPQ - Simulation and Optimisation of Chemical Processes

Last modified: 02/10/2025

Unit in charge: Barcelona East School of Engineering
Teaching unit: 713 - EQ - Department of Chemical Engineering.

Degree: BACHELOR'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Compulsory subject).

Academic year: 2025 **ECTS Credits:** 6.0 **Languages:** Catalan

LECTURER

Coordinating lecturer: MOISES GRAELLS SOBRE

Others: Primer quadrimestre:
ALBA ÁGUEDA COSTAFREDA - Grup: T1
MOISES GRAELLS SOBRE - Grup: T1

PRIOR SKILLS

Sufficient capacity of written communication. Autonomous learning.

REQUIREMENTS

OPERACIONS BÀSIQUES I - Prerequisit
OPERACIONS BÀSIQUES II - Corequisit

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
2. Analyse, design, simulate and optimise processes and products.

Transversal:
1. EFFECTIVE USE OF INFORMATI0N RESOURCES - Level 3. Planning and using the information necessary for an academic assignment (a final thesis, for example) based on a critical appraisal of the information resources used.

TEACHING METHODOLOGY

The course uses lecturing by 20%, group work in the classroom 20%, individual work 20%, work in groups by 20%.
Competence in the solvent use of information resources, which is the competence to be assessed in this course is examined in the course simulation project, as well as in the partial and final exams.

LEARNING OBJECTIVES OF THE SUBJECT

Know how to systematically formulate steady state mass and energy balances.
Know how to prepare efficient calculation schemes for automatically solving mass and energy balances (ideal / linear) in stead state using a spreadsheet (Excel).
Know how to prepare efficient calculation schemes for automatically solving mass and energy balances (ideal / linear) in steady state using algebraic modeling languages â□□â□□(GAMS).
Identify and explain the sequential-modular approach and the equation-oriented approach.
Know how to incorporate numerical methods for the calculation of thermodynamic and transport properties (non-ideal / non-linear) by programming the spreadsheet (Excel VBA).
Know how to find solvent information on thermodynamic properties, and select and adjust thermodynamic models reproducing the experimental behavior of mixtures (ELV).
To know how to simulate complex processes in the stationary state using several commercial simulators of chemical processes (UniSim, VMGSim, AspenHYSYS, AspenPlus, etc.)

STUDY LOAD

Type	Hours	Percentage
Hours small group	30,0	20.00
Hours large group	30,0	20.00
Self study	90,0	60.00

Total learning time: 150 h

CONTENTS

(ENG) Tema 1. Introducció

Description:
(ENG) Modelització, simulació, optimització i presa de decisions. Definicions: Model, variable, paràmetres, restriccions i funció objectiu. Limitació dels models. El temps de càlcul com a variable del problema. Càlculs preliminars: estimacions, acotacions y heurístiques. Exercicis.

Specific objectives:
(ENG) Aprendre a modelitzar, analitzar i a simular processos químics en estat estacionari. Aprendre a programar funcions d'usuari per a la resolució numèrica de les equacions dels models i per al càlcul de propietats termodinàmiques. Aprendre a ajustar els paràmetres d'un model.

Related activities:
(ENG) Exercicis de supòsits relacionats amb el contingut del tema, realitzats amb suport Excel.

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) Tema 2.

Description:
Spreadsheet. Justification for the use of this tool. User interface. Control variables, parameters and constraints. Macro programming. Degrees of freedom. Limitations of the model. Exercises.

Specific objectives:
Learning to model, analyze and simulate chemical processes in steady state. Learn to program user functions for the numerical solution of the equations and models to calculate thermodynamic properties. Learn to adjust the parameters of a model.

Related activities:
Practical case exercises related to the content of this chapter, made on Excel.

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) Tema 3.

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) -

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) -

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) -

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) -

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) -

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) -

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

(ENG) -

Full-or-part-time: 8h
Theory classes: 3h
Self study : 5h

GRADING SYSTEM

1. Problems 25%
2. Partial Exam 25%
3. Final Exam 25%
4. Simulation Project 25%. There is no re-evaluation exam.

EXAMINATION RULES.

Exams will be performed individually in the computer room. Exams will consist in the preparation of solutions to process simulation problems, and will be presented in a digital format through ATENEA within the time-frame prescribed.

BIBLIOGRAPHY

Basic:

- Skogestad, Sigurd. Chemical and energy process engineering. Boca Raton: CRC Press, cop. 2009. ISBN 9781420087550.
- Ghasem, Nayef; Henda, Redhouane. Principles of chemical engineering processes. Boca Raton, FL: CRC Press, cop. 2009. ISBN 9781420080131.
- Gmehling, Jürgen; Kleiber, Michael; Kolbe, Bärbel; Bärbel, Jürgen. Chemical thermodynamics for process simulation. Second edition. Weinheim, Germany: Wiley, 2019. ISBN 9783527343256.
- Finlayson, Bruce A. Introduction to chemical engineering computing. Hoboken, N.J: Wiley Interscience, cop. 2006. ISBN 0471740624.
- Gil Chaves, Iván Darío; López, Javier Ricardo Guevara; García Zapata, José Luis; Leguizamón Robayo, Alexander; Rodríguez Niño, Gerardo. Process Analysis and Simulation in Chemical Engineering [on line]. Cham: Springer International Publishing, 2016 [Consultation: 30/06/2023]. Available on: https://discovery.upc.edu/permalink/34CSUC_UPC/rdgucl/alma991004876355706711. ISBN 3319148125.

Complementary:

- Arpe, Hans-Jürgen. Industrial organic chemistry. 5th completely revised ed. Weinheim, Germany: WileyVCH, 2010. ISBN 9783527320028.
- Shreve, Randolph Norris; Austin, George T. Shreve's chemical process industries. 5th ed. New York [etc.]: McGraw-Hill Book Company, cop. 1984. ISBN 0070571473.
- Kent, James Albert. Kent and Riegel’s Handbook of Industrial Chemistry and Biotechnology [on line]. Eleventh Edition. Boston, MA:

Springer US, 2007 [Consultation: 20/09/2023]. Available on: https://discovery.upc.edu/permalink/34CSUC_UPC/rdgucl/alma991001811119706711. ISBN 9780387278438.