Course guide
320069 - SOCPQ - Simulation, Optimization and Control of Chemical Processes

Unit in charge:	Terrassa School of Industrial, Aerospace and Audiovisual 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:	Antoni Escalas Cañellas
Others:	Antoni Escalas Cañellas Manuel Carrasco Portero

PRIOR SKILLS

In order to be able to follow the course properly, it's essential to have passed the courses of Fundamentals of Chemical Engineering (Q4) and Control and industrial automation (Q4). Since in this SOCPQ course you are going to model process units such as pumps, valves, chemical reactors, heat exchangers, distillation and gas absorption columns, etc., it is important for you to have taken the subjects Unit Operations 1 (Q5) and Chemical Reaction Engineering (Q5) and to be enrolled in the subject Unit Operations 2 (Q6).

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
CE20. CHE: ability to analyse, design, simulate and optimise processes and products.

CE22. CHE: Ability to design, manage and operate procedures for the simulation, control and instrumentation of chemical processes.

CE19. CHE: Knowledge of material and energy balances, biotechnology, the transfer of materials, separation operations, chemical reaction engineering, the design of reactors, and the reuse and transformation of raw materials and energy resources.

Transversal:
07 AAT N3. SELF-DIRECTED LEARNING - Level 3. Applying the knowledge gained in completing a task according to its relevance and importance. Deciding how to carry out a task, the amount of time to be devoted to it and the most suitable information sources.

TEACHING METHODOLOGY

- Presentation classroom sessions by the lecturer.
- Application classroom sessions, practical work in the classroom
- Practical laboratory sessions .
- Autonomous study and exercises.
- Completion of an independent project simulation in Aspen or, otherwise, in the chemical process simulation program chosen by the professor.
- Completion of independent Control and Automation projects

In presentation sessions the lecturer expands the theoretical basis of the material already seen in " Industrial Control and Automation " , focusing on applications in chemical processes . We also introduce the concepts and methods of simulation and process optimization illustrating them with examples appropriate to facilitate understanding .

Practical sessions in the classroom will be of two kinds:
a) sessions in which the lecturer guides students to analyze data and solve problems by applying techniques , concepts and theoretical results .
b) examination sessions and / or presentation of work

Practical laboratory work sessions will include:
- Simulation laboratory sessions where chemical operations and processes will be designed and optimized from the simulation software Aspen or, otherwise, in the chemical process simulation program chosen by the professor.- Control and Automation laboratory sessions, where different process control systems will be designed and implemented, with the help of Matlab / Simulink (or similar) type software and micro PLCs and the necessary instrumentation.

Simulation project - Self-directed learning
Each couple of students will be assigned an individual project simulation of chemical processes with Aspen or, otherwise, in the chemical process simulation program costen by the professor, to be developed independently throughout the semester. This project will be developed primarily outside the classroom, though 2-3 laboratory sessions (mostly during the 2nd bimester) will be devoted to student work on the project, supervised by the lecturer.

LEARNING OBJECTIVES OF THE SUBJECT

· To familiarise students with the techniques of prediction and estimation and data optimization techniques .
· To develop the student's ability to apply these techniques wisely .
· To introduce students to the techniques of control chemical processes themselves .
· To introduce students to different commercial softwares to simulate the chemical processes from the design stage to the control and optimization.
· To develop specific skills associated with academic and transverse detailed below.
Specific skills :
· Ability to design , manage and operate procedures for simulation , control and instrumentation for chemical processes .
· Ability to implement process optimization and chemicals.
· Ability to design and implement in a practical way regulation and control systems of basic process units and / or real complete chemical plants.
· Knowledge and application of the terminology used to describe the concepts relevant to this matter.

Generic skills:
· Ability to formulate and solve problems
· Critical reasoning
· Autonomous learning
· Ability to work in group
· Time management and organization of work
· Ability to write and develop projects

STUDY LOAD

Type	Hours	Percentage
Hours small group	15,0	10.00
Self study	90,0	60.00
Hours medium group	15,0	10.00
Hours large group	30,0	20.00

Total learning time: 150 h

CONTENTS

T1. INDUSTRIAL CONTROL APPLIED TO CHEMICAL PROCESSES

Description:
Application of Process Control to chemical engineering and its operations:

1.- Continuous Control:
Feedback control.
Feedforward control.
Feedforward-feedback control.
Relationship control.
Cascade control.
Auction control.
Inferential control
Other control systems: Fuzzy logic, Robust, Statistical, Predictive control, Adaptive control,
Optimization of control systems.
Offline, real-time optimization, neural networks and expert systems.

2.- Control of discrete processes:
- The Programmable Automaton
- Programming languages:
- Graphic languages: Ladder, GRAFCET
- Structured Text Languages ST (Language C).

3.- SCADA: Monitoring, control and data capture systems
4.- Practical implementation of process control systems.
- Practical implementation of Process Control Systems with Arduino micro PLCs and Matlab / Simulink software or similar.

Specific objectives:
- The ability to apply the control techniques covered in this subject to chemical processes.
- An understanding of feedforward systems.
- An understanding of control systems based on examples.
- The ability to optimise control systems.
- The ability to design and implement control keys and simple SCADA systems in a practical way with adequate hardware and software.

Full-or-part-time: 75h
Theory classes: 30h
Self study : 45h

T2. PROCESS SIMULATION

Description:
- Prediction of physical and chemical properties in single-component systems.
- Equations of state.
- Multicompone- Prediction of physicochemical properties in one-component systems.
- State equations.
- Multicomponent systems.
- Prediction of thermodynamic properties.
- Application of predictive models in the processs simulation software.
- Design of unit operations in the process simulation software
- Design of a process in the process simulation software
- Design of process control in the process simulation software
- Other simulation programs

Specific objectives:
- To learn the basics of predictive models used in simulation programs on the market.
- To know how to interpret the validity of the available data according to their origin.
- To relate the different physicochemical and thermodynamic properties.
- To Estimate the value of properties not available.
- To work with the Aspen software (or other program chosen by the professor).
- To provide an overview of the possibilities of process simulation as a tool for computer systems analysis, which minimizes risks and costs in experimentation.

Related activities:
- Introduction to simulation software of choice, and development of real processes and operations.
- Simulation laboratory practices
- Development of an individual project

Full-or-part-time: 51h
Practical classes: 10h
Laboratory classes: 10h
Self study : 31h

T3. PROCESS OPTIMISATION

Description:
- Introduction to Optimisation. Optimisation in Chemical Engineering
- Theory and optimisation algorithms: Constrained/Unconstrained Optimisation
- Linear / nonlinear problems
- Linear programming, simplex method, nonlinear programming
- Process simulation and its link to optimisation.

Specific objectives:
- Developing the ability to recognise and solve situations requiring the use of optimisation tools.
- Obtaining knowledge on mathematical optimisation algorithms and their application
- Using computer optimisation tools.
- Offer a range of optimization techniques able to solve many problems that can arise in Chemical Engineering.

Related activities:
- Application of the simulation software, and other, to the optimization of real processes and operations.

Full-or-part-time: 24h
Practical classes: 5h
Laboratory classes: 5h
Self study : 14h

GRADING SYSTEM

ORAL AND WRITTEN TESTS 50%:
- Mid-term Simulation exam 12.5%, eliminatory character
- Mid-term Automation & Control exam, 12.5%, eliminatory character
- Final Optimization exam 12.5%
- Final Automation & control exam 12.5%

50% PRACTICAL PROJECTS AND WORKS:
Simulation Laboratory (Aspen or other software chosen by the professor) 5%
Simulation project (Aspen or other software chosen by the professor) 20%
8% Automation and Control Project
11% Automation & Control laboratory practices
6% Automation & Control deliverable tasks

* Obligation to make and deliver projects and practical works *
On the basis of paragraph 3.1.3 of the General Academic Standard, we have established in this course that it is a necessary condition for passing the course to have carried out the projects and practical works, and have submitted the corresponding reports. This condition will apply to students who, unjustifiably at the teacher's discretion, have not done and delivered at least 90% of the set of projects and practical work, a percentage that will be calculated with the sum of weightings assigned to the parts of projects+practical works effectively done and delivered. In this case, the final grade for the subject that will be applied will be "Not Presented".

Note: The simulation project and the control and automation tasks also serve for the assessment of the "Autonomous Learning" skill.

- This course has no resit because it does not have any evaluation act weighing more than 25%.
- This subject has a re-assessment exam (June/July), in accordance with the ESEIAAT assessment regulations. For those students who meet the requirements and take the reassessment exam, the grade from the reassessment exam will replace the grades of all the assessment acts that are face-to-face written tests (controls, partial and final exams) and the grades of practices, work, projects and presentations obtained during the course.

If the final grade after the reassessment is less than 5.0, it will replace the initial grade only if it is higher. If the final grade after the reassessment is greater than or equal to 5,0, the final grade for the course will be approved 5.0.

EXAMINATION RULES.

Bring to the exam:
- Blank A4 sheets; blue or black pen to answer the exam
- A calculator with all the necessary mathematical functions and which, in addition, can solve implicit equations and find the zeros of polynomials and other mathematical functions.
- The formulary that the professor will publish on Atenea for each exam, and only this formulary.
- The graphs and tables indicated by the professor (Athena)

BIBLIOGRAPHY

Basic:
- Poling, Bruce E.; Prausnitz, John M.; O'Connell, John P. The properties of gases and liquids. 5th ed. New York [etc.]: McGraw-Hill, cop. 2001. ISBN 0070116822.
- Ramirez, W. Fred. Computational methods for process simulation [on line]. 2nd ed. Boston: Butterworths, 1997 [Consultation: 09/07/2024]. Available on: https://www-sciencedirect-com.recursos.biblioteca.upc.edu/book/9780750635417/computational-methods-in-process-simulation. ISBN 075063541X.
- Bequette, B. Wayne. Process dynamics : modeling, analysis and simulation. Upper Saddle River: Prentice-Hall, 1998. ISBN 0132068893.
- Stephanopoulos, George. Chemical process control : an introduction to theory and practice. Wilmington: Prentice-Hall, 1984. ISBN 0131285963.
- Bateson, Robert N. Introduction to control system technology. 7th ed. Upper Saddle River ; Columbus: Prentice Hall, 2001. ISBN 0130306886.
- Ollero de Castro, Pedro. Control e instrumentación de procesos químicos. Madrid: Síntesis, 1997. ISBN 8477385173.

Complementary:

- Crowe, C. M. Chemical plant simulation : an introduction to computer-aided steady-state process analysis. Hamilton: McMaster University, 1969. ISBN 0131286862.
- Colbourn, Elizabeth A. Computer simulation of polymers. New York: Longman Scientific & Technical, 1994. ISBN 0582083745.
- Smith, Carlos A.; Corripio, Armando B. Control automático de procesos : teoría y práctica. México: Limusa, 1996. ISBN 9789681837914.
- Mayol i Badia, Albert. Autómatas programables. Barcelona: Marcombo, 1987. ISBN 842670672X.
- Shinskey, F. Greg. Process control systems: application, design and tuning. 4th ed. New York: McGraw-Hill, 1996. ISBN 0070571015.
- Creus Solé, Antonio. Instrumentación industrial [on line]. 8a ed. Barcelona: Marcombo, 2011 [Consultation: 19/09/2022]. Available on: https://www-ingebook-com.recursos.biblioteca.upc.edu/ib/NPcd/IB_BooksVis?cod_primaria=1000187&codigo_libro=9767. ISBN 9788426731890.
- Medina, José Luis. La automatización en la industria química [on line]. Barcelona: Edicions UPC, 2010 [Consultation: 12/05/2020]. Available on: http://hdl.handle.net/2099.3/36842. ISBN 9788498803983.

RESOURCES

Other resources:

- Guadayol Cunill, Josep Maria. Control, instrumentació i automatització de processos químics: problemes [en línia]. Barcelona: Edicions UPC, 1999 [Consulta: 10/03/2008]. Disponible a: <http://bibliotecnica.upc.es/EdUPC/locate4.asp?codi=QU005XXX>. ISBN 84-8301-310-X.
- Aspen Plus User's Manual online. Available et: https://web.ist.utl.pt/ist11038/acad/Aspen/AspUserGuide10.pdf />- Diverse authors. Tutorials. [DWSIM tutorials at the DWSIM Wiki]. Available at http://dwsim.inforside.com.br/wiki/index.php?title=Tutorials. />- DWSIM forums at Sourceforge. Available at https://sourceforge.net/p/dwsim/discussion/