COURSE DATA

Data Subject	
Code	44435
Name	Simulation and advanced optimisation of processes
Cycle	Master's degree
ECTS Credits	6.0
Academic year	2023 - 2024

Study (s)

Degree	Center	Acad. year	Period
2209 - M.D. in Chemical Engineering	School of Engineering	1	Second term

Subject-matter

Degree	Subject-matter	Character
2209 - M.D. in Chemical Engineering	8 - Simulation and advanced optimisation of processes	Obligatory

Coordination

Name	Department
BORRAS FALOMIR, LUIS	245 - Chemical Engineering
RIBES BERTOMEU, JOSEP	245 - Chemical Engineering
RUANO GARCIA, MARIA VICTORIA	245 - Chemical Engineering

SUMMARY

The main objective of the subject Advanced Process Simulation and Optimization is to let the students know the methodology that is used to develop unit operations models in Chemical Engineering. They will be able to apply these models properly to process simulation and optimization.

The subject is divided in two parts. During the first part, the analysis and model calibrations procedures will be studied. The acquired knowledge will be applied by using the software Matlab®. In the second part, the models will be applied to the simulation of specific industrial processes, either under steady state or dynamic, for the equipment dimension and process optimisation. During this part, several case studies will be solved by using the commercial simulators Aspen Plus® and Aspen Hysys®.

It is a semester mandatory subject taught during the second semester of the Master in Chemical Engineering. At the present curriculum, it consists of 6 ECTS. This subject is part of the general module “Product and Processes Engineering” which is made up of a total of 45 ECTS.

The subject will be taught in Spanish.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

OUTCOMES

2209 - M.D. in Chemical Engineering

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Be able to apply the scientific method and the principles of engineering and economics to formulate and solve complex problems in processes, equipment, facilities and services in which matter changes its composition, state or energy content, these changes being characteristic of the chemical industry and of other related sectors such as pharmacology, biotechnology, materials science, energy, food or the environment.
- Conceive, plan, calculate and design processes, equipment, industrial facilities and services in the field of chemical engineering and other related industrial sectors in terms of quality, safety, economics, rational and efficient use of natural resources and environmental conservation.
- Know how to establish and develop mathematical models by using appropriate software in order to provide the scientific and technological basis for the design of new products, processes, systems and services and for the optimisation of others already developed.

- Integrate knowledge and handle the complexity of formulating judgments and decisions, based on incomplete or limited information, which take account of the social and ethical responsibilities of professional practice.
- Communicate and discuss proposals and conclusions in specialised and non-specialised multilingual forums, in a clear and unambiguous manner.
- Adapt to changes and be able to apply new and advanced technologies and other relevant developments with initiative and entrepreneurship.
- Have skills for independent learning in order to maintain and enhance the specific competences of chemical engineering which enable continuous professional development.
- Be able to access information tools in different areas of knowledge and use them properly.
- Be able to assess the need to complete their technical, scientific, language, computer, literary, ethical, social and human education, and to organise their own learning with a high degree of autonomy.
- Be able to defend criteria with rigor and arguments and to present them properly and accurately.
- Be able to take responsibility for their own professional development and specialisation in one or more fields of study.
- Design products, processes, systems and services for the chemical industry and optimise others already developed, on the basis of the technologies of various areas of chemical engineering including transport processes and phenomena, separation operations and engineering of chemical, nuclear, electrochemical and biochemical reactions.
- Apply critical reasoning to their knowledge of mathematics, physics, chemistry, biology and other natural sciences, obtained through study, experience and practice, in order to establish economically viable solutions to technical problems.
- Conceptualize engineering models; apply innovative methods in problema solving and applications suitable for the design, simulation, optimization and control of processes and systems.
- Be able to solve unfamiliar and ill-defined problems that have specifications in competition by considering all possible methods of solution, including the most innovative ones, and selecting the most appropriate, and correct implementation by evaluating the different design solutions.
- Direct and supervise all types of facilities, processes, systems and services in different industrial areas related to chemical engineering.

LEARNING OUTCOMES

Know the different types of models, stationary and dynamic to simulate for Chemical Engineering process.

Be able to develop mathematical models and estimate the value of the parameters from experimental data and assessing the fit obtained.

Know the mathematical optimization algorithms most used and be able to apply to specific cases using numerical calculation tools.

Be able to carry out a sensitivity and uncertainty analysis of a mathematical model and draw conclusions.

Know the models to estimate thermodynamic properties commonly used in Chemical Engineering.

Understand and acquire skill in the use of simulators for design of basic equipment used in chemical plants.

Be able to optimize the performance of a complete chemical plant using simulators (including the integration of both process and energy streams) and to present the results.

DESCRIPTION OF CONTENTS

1. Mathematical modelling in process simulation and optimization.

Simulation of chemical processes: stationary and dynamic models. Model formulation. Uncertainty and sensitivity parameters. Analysis of global and local sensitivity.

Parameter estimation. Method of least squares for the calibration of parameters. Advanced optimization algorithms. Estimation of uncertainty in the parameters.

Using tools for parameter estimation and optimization. Development of complex simulation models in Matlab. Calculating the sensitivity of the parameters. Getting the most important parameters. Application of advanced optimization algorithms for parameter estimation: Genetic algorithms and other search techniques.

2. Process design and simulation using Aspen Plus® y Aspen Hysys®

Simulation in steady state and dynamic. Selection and application of prediction models of thermodynamic properties. Design of industrial processes. Optimization. Sizing equipment. Introduction to the use of Aspen Process Economic Analyzer® (ACEP). Resolution of practical cases.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Laboratory practices	16,00	100
Seminars	10,00	100
Classroom practices	10,00	100
Tutorials	4,00	100
Development of group work	40,00	0
Development of individual work	10,00	0
Study and independent work	20,00	0
Preparation of evaluation activities	10,00	0
Preparation of practical classes and problem	10,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

The course will be developed through lectures and practical classes.

Classroom sessions: through participatory lectures, the main concepts will be developed to provide a comprehensive and integrated vision, analysing in detail the key and most complex aspects, promoting, at all times, student participation. Adequate resources for further preparation of the subject in depth by the student will be also recommended.

Practical activities: The practical sessions will complement the theoretical activities in order to apply the basics, and expand the knowledge and experience that the students acquired during the fulfilment of the proposed work. This will be done in the classroom or in small groups. The following types of classroom activities are included:

- Classes of exercises and questions in the classroom. The teacher will explain a number of standard exercises, which allow students to acquire the necessary skills to analyse, formulate and solve the problems of each subject. Some problems will be solved in practical sessions in small groups.
- Sessions for discussion and resolution of exercises. In these sessions the students will analyse and discuss a series of exercises or work previously posed by the teacher. These sessions will be conducted in small groups.
- Practices in the computer classroom. In these sessions, students will use the commercial simulators Aspen HYSYS® and Aspen Plus® for the practical application of knowledge and skills developed during the course, to design, simulation and optimization. These sessions will be conducted in small groups.

For the development of all these activities, both students and the teacher will use the “Aula Virtual” platform.

EVALUATION

For the assessment of the student learning it will be considered the continuous evaluation, an evaluation of practical activities and a final evaluation using two methods:

Method A:

ITEM	% OVER FINAL MARK
Classroom activities	5
Deliverable project	60
Final exam	35

Method B:

ITEM	% OVER FINAL MARK
Classroom activities	5
Deliverable project	45
Final exam	50

To be eligible for mode A, a minimal attendance of 90% at practice sessions is required.

Classroom activities: It will be based on participation and student involvement in the teaching/learning process, taking into account regular attendance at the planned classroom activities, and the resolution of proposed questions, individually and/or in small groups.

Deliverable project: It will be based on the resolution of a case by using the process simulator, and the development of a detailed report including all aspects worked on the computer sessions.

Final exam: The student must make an individual objective test, which consist of an examination at the end of the course. This exam will consist of both theoretical/practical questions and exercises, in order to ascertain whether they have assimilated the basic concepts of the subject.

The minimum mark to pass the subject will be 5 out of 10, whenever a mark equal to or greater than 5 points (out of 10) in the deliverable project and the final exam is obtained.

The assessment system is independent of the call (1st or 2nd).

REFERENCES

Basic

- Nicolás J. SCENNA y col., 2007, Modelado, simulación y optimización de procesos químicos, Edutecne.
- Edgar, T. F., Himmelblau, D. M. and Lasdon, L. S., 2001. Optimization of Chemical Processes, McGraw-Hill.
- SEIDER, W.D, SEADER, J.D., LEWIN, D.R., 1999. Process Design Principles, John Wiley & Sons, New York

Additional

- Steven C. Chapra y Raimond P. Canale, 1988. Métodos Numéricos para Ingenieros. McGraw-Hill, México.
- Ravindran, A., Ragsdell, K. M., Reklaitis, G. V., 2007. Engineering Optimization: Methods and Applications, John Wiley & Sons, New York.
- LUYBEN, W.L, 2006, Distillation design and control using Aspen Simulation, John Wiley & Sons, New York