Universidad del País Vasco Euskal Herriko Unibertsitatea

COURSE GUIDE 2024/25

Faculty 310 - Faculty of Science and Technology **Cycle** .

Degree INQUI15b - Master in Chemical Engineering **Year** .

COURSE

504254 - Advanced optimization of chemical processes **Credits, ECTS:** 4,5

COURSE DESCRIPTION

In today's world, where success is associated with being highly busy, almost all of our actions and decisions seek maximum efficiency, i.e., they seek the best possible way to achieve them: optimus (best), izare (convert into). Managing a company is, in itself, a problem of optimization. Companies try to balance cost minimization with other factors that maximize the company's profitability in a way that provides competitive advantage. Optimization covers practically all areas of the company: finance and banking, logistics and transportation, supply chain, process design, production management, insurance and reinsurance, energy and raw material consumption, personnel organization, etc.

Optimal decisions must respect the logical constraints of real life (economic-financial, market, physical and chemical, thermodynamic, environmental, security, rights, etc.), which ensures that solutions are feasible.

The first optimization methods date back to the time of Isaac Newton (1643-1727), Joseph-Louis Lagrange (1736-1813) and Augustin-Louis Cauchy (1789-1857), but the real progress in mathematical theory and practical implementation of optimization came in the middle of the 20th century, with the development of computers.

The first stage of this optimal design process is the identification of an opportunity for improvement, in which the creativity and imagination of the individual is the most important factor.

The second stage consists of modeling the previously identified problem through a process of abstraction and the assumption of consistent hypotheses, generating a mathematical model that represents reality well.

The third stage in the optimal design process is to solve this mathematical optimization model by means of appropriate algorithms and/or using available software.

The fourth and final stage consists of analyzing the results obtained and reviewing the validity of the hypotheses assumed, always bearing in mind that optimization is a process of continuous improvement that should never end.

That said, the main objective of the course is, hence, to model and solve production improvement problems of a chemical process, or other related processes in the field of engineering. There is no single optimization method that can efficiently solve all types of problems and hence various methods have been developed over the years. In this course, priority will be given to algorithmic and implementation aspects over theoretical aspects. Therefore, good programming skills are required, as well as basic knowledge of calculus and trigonometry. The syllabus is divided into 4 sections: linear programming, integer programming, nonlinear programming and design of experiments oriented to process optimization.

COMPETENCIES/LEARNING RESULTS FOR THE SUBJECT

COMPETENCIAS DE LA ASIGNATURA

Apply knowledge of mathematics, physics, chemistry, biology, and other natural sciences, obtained through study, experience, and practice, with critical reasoning to establish economically viable solutions to technical problems.
To design products, processes, systems and services for the chemical industry, as well as the optimization of others already developed, taking as a technological base the different areas of chemical engineering, including processes and transport phenomena, separation operations and chemical, nuclear, electrochemical and biochemical reaction engineering.
Conceptualize engineering models, apply innovative problem-solving methods and appropriate computer applications for the design, simulation, optimization and control of processes and systems
Manage and supervise all types of installations, processes, systems and services in the different industrial areas related to chemical engineering.

RESULTADOS DE APRENDIZAJE DE LA ASIGNATURA

- Identify and simplify an optimization problem in the field of chemical engineering.
- Perform a cost-benefit trade-off analysis.
- Select and implement the proper optimization method for solving each problem.
- Apply material and energy balances, transfer equations (matter, energy and quantity of motion), and equilibrium equations to model and simulate separation and chemical reaction operations of the optimization problem.
- Model and simulate separation and chemical reaction operations using calculation programs (Matlab, Scilab, Gams) and process simulation programs (PRO/II, Aspen, Hysys, etc.), on which the optimization calculation can be performed.
- Plan a set of tests to optimize systems or processes for which insufficient information is available.
- Analyze the result: check its feasibility and analyze its sensitivity to the assumptions made, to the uncertainties of

the context and to the decision variables.
- Communicate by means of a written report the creation, development of the scenario and its results in an effective way (contextualized, balanced, hierarchical and structured, clear, impacting, with language correction and adequate linguistic register and appropriate conventions: formats, titles, captions, legends,...).
- Communicate through effective oral presentation (contextualized, balanced, hierarchical and structured, clear, impacting), the creation, elaboration of the case and its results in a limited time.
- Establish and assume responsibilities for the teams' management (rules of operation, distribution of tasks, control of dates, active participation, ...).
- Self-evaluate the team's performance to enhance efficiency and collaboration for the next assignments.

Theoretical and Practical Contents

INTRODUCTION: Formulation of an optimization problem; types of problems. Review of basic techniques.
LINEAR PROGRAMMING: Problem definition. Simplex Algorithm. Examples and applications in Chemical Engineering.
NON-LINEAR PROGRAMMING: Problem definition. Nelder and Mead algorithm. Gradient-based methods. Examples of regression application. Applications to Chemical Engineering.
INTEGER PROGRAMMING: Problem definition. Branching and dimensioning method. Dynamic programming. Practical examples.
DESIGN OR EXPERIMENTS: Design of optimization experiments. Advantages of experimental design. Minimum squares for linear models. Introduction to EVOP techniques. Examples.

METODOLOGIA (ACTIVIDADES FORMATIVAS)

Actividad Formativa	Hours	Porcentaje presencialidad
Presentation and defence of projects	5	100 %
Exercises	10	20 %
Expositive classes	15	100 %
Handling sources and resources	17,5	0 %
Groupwork	30	30 %
Case analysis	35	40 %

TYPES OF TEACHING

Types of teaching	M	S	GA	GL	GO	GCL	TA	TI	GCA
Hours of face-to-face teaching	15				30				
Horas de Actividad No Presencial del Alumno/a	20				47,5				

Legend:
M: Lecture-based
S: Seminar
GA: Applied classroom-based groups
GL: Applied laboratory-based groups
GO: Applied computer-based groups
GCL: Applied clinical-based groups
TA: Workshop
TI: Industrial workshop
GCA: Applied fieldwork groups

Evaluation tools and percentages of final mark

Denominación	Ponderación mínima	Ponderación máxima
Written examination	0 %	50 %
Presentations	20 %	60 %
Practical tasks	40 %	70 %

ORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

Assessment in ordinary call is based on three types of tasks:

1) Elaboration of four optimization cases (linear, integer, non-linear and design of experiments) in teams, which will be graded in relation to the learning outcomes, attending to their originality, degree of difficulty, appropriateness, coherence, resolution, and their written presentation, as well as under criteria of involvement in the team. The four optimization cases are presented in a staggered manner throughout the course (weeks 5, 7, 10 and 13).

2) Oral presentation of one of the four cases, which will be evaluated according to the common criteria for effective presentations.

3) An individual test, which consists of analyzing and evaluating an optimization case presented by other students and providing feedback. The test will be graded in relation to the handling and justification of the criteria established in (1). Minimum grade: 5

The call may be renounced before week 10 of the teaching period. This renunciation must be presented in written form to the professors. The renunciation implies that it will not be counted (not presented).

EXTRAORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

The assessment in the extraordinary call will consist of three elements similar to the ordinary call:

1) Elaboration of an optimization case, which will be graded in relation to the learning outcomes, attending to its originality, degree of difficulty, adequacy, coherence, resolution, and its written presentation.

2) Oral presentation of the case, which will be evaluated according to the common criteria for effective presentations.

3) An individual test, which consists of analyzing and evaluating an optimization case presented by other students and providing feedback. The test will be graded in relation to the handling and justification of the criteria established in (1). Minimum grade: 5

MANDATORY MATERIALS

Matlab

BIBLIOGRAPHY

Basic bibliography

Edgar, T.F., Himmelblau, D.M., Optimization of Chemical Processes, 2nd edition. McGraw-Hill, 2002.
Box, G.E., Hunter, J.S., Hunter, H.G. Statistics for Experimenters: Design, Innovation, and Discovery, 2nd edition. Wiley, 2005.
Biegler L.T., Nonlinear Programming: Concepts, Algorithms and Applications to Chemical Processes. MOS-SIAM, 2010.
Turton, R., Bailie, R.C., Whiting, W.B., Shaeiwitz, J.A., Bhattacharyya, D., Analysis, Synthesis and Design of Chemical Processes, 4th edition. Pearson, 2013.
Peters, M.S., Timmerhaus, K.D., West, R.E., Plant Design and Economics for Chemical Engineers, 5th edition. McGraw-Hill, 2013.

Detailed bibliography

Douglas, J.M., Conceptual Design of Chemical Processes, Chem. Eng. Series, McGraw-Hill, 1988.
Taguchi, G., Introduction to Quality Engineering. Designing Quality into Products and Proceses, Quality Resources, 1990.

Journals

Industrial & Engineering Chemistry Research
Chemical Engineering Science
Chemical Engineering Processing

Web sites of interest