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

504255 - Modelling and simulation of chemical processes **Credits, ECTS:** 6

COURSE DESCRIPTION

This subject is a core subject from the Chemical Engineering field and therefore it is mandatory, like in any other Chemical Engineering Master’s Degree in Spain or around the world. In order to take advantage of the course, it is necessary to have studied the basic subjects of Chemical Engineering. This includes subjects that deal with transport phenomena (Fluid Mechanics, Heat Transfer, and Mass Transfer), as well as those that deal with the design of chemical reactors (Kinetics of Chemical Processes and Reactor Design) and separation processes (Separation Processes). Moreover, it is recommended to have knowledge of the following subjects: Numerical Methods, Thermodynamics, Instrumentation and Control of Chemical Processes, and Programming. All of these subjects are included in the Chemical Engineering Bachelor Degree in addition to many other technical Bachelor Degrees. The knowledge and use of scientific programming languages such as Scilab and Matlab or that of process simulation in steady state (Pro II, ASPEN, HYSIS, or DWSIM) is desirable, but not imperative. The subject is closely related to all the contents from the Master’s that broaden the knowledge of the foundations of Chemical Engineering: Advanced Chemical Reactors, Advanced Process Control, Advanced Separation Processes, and Advanced Optimization of Chemical Processes.

Studying and passing this subject provides the student with the ability to approach the modelling and simulation of non-steady physic-chemical processes of industrial interest, using the calculus capacity of microprocessors to build tools that give way to address the effect of the design variables and those of operation conditions on the results of the process. The possibilities to actually apply the knowledge acquired in this subject in real professional practice are then unlimited.

COMPETENCIES/LEARNING RESULTS FOR THE SUBJECT

COMPETENCIAS DE LA ASIGNATURA

Application of the knowledge from Mathematics, Physics, Chemistry, Biology, and other natural sciences obtained from their studies, experience, and practice, using critical thinking to establish technical solutions that are viable from the economic point of view

Design of products, processes, systems, and services of the chemical industry, as well as the optimization of others that have already been developed, based on the diverse areas of Chemical Engineering: process understanding, transport phenomena, separation processes, and chemical, nuclear, electrochemical, and biochemical reactions.electroquímicas y bioquímicas

To conceptualize engineering models, apply innovative methods in the resolution of problems and the application of proper computer applications for the design, simulation, optimization and control of the processes and the systems

To have the ability to solve non-familiar problems, not-completely defined, and have competing specifications, considering the multiple ways of solution, including the most innovative ones, choosing the best and evaluating the different design solutions.

RESULTADOS DE APRENDIZAJE DE LA ASIGNATURA

After completing the course, students should be able to:
- Identify the fundamental phenomena that control a process
- Develop the mathematical model that describes a process
- Solve the equations by means of advanced calculus tools
- Evaluate the suitability of the developed model based on the analysis of the results
- Propose and implement diverse situations and pondering of the model¿s response

Theoretical and Practical Contents

Mass and Momentum balances in steady and non-steady state. Transfer in the interface. Microscopic Mass and Momentum balances in steady and non-steady state: equation of continuity. Velocity profiles.
Macroscopic Energy Balances in steady and non-steady state. Transfer in the interface.
Microscopic Energy Balances: temperature profiles in solid and fluid mediums.
Macroscopic and Microscopic Mass Balances in multicomponent systems. Concentration profiles with one or more independent variables. Transfer in the interface.
Macroscopic and Microscopic Mass Balances in multicomponent systems with chemical reactions. Inclusion of the kinetic model to the Mass balance. Concentration profiles with one or more independent variables. Numerical methods for the resulting equations of the modelling: multiple linear equations, multiple non-linear equations, ordinary differential equations, and partial differential equations.
Preparation of the developed model by computer software for evaluation and external use.

METODOLOGIA (ACTIVIDADES FORMATIVAS)

Actividad Formativa	Hours	Porcentaje presencialidad

Presentation and defence of projects	6	100 %
Expositive classes	12	100 %
Handling sources and resources	17	0 %
Groupwork	30	40 %
Case analysis	40	30 %
Exercises	45	40 %

TYPES OF TEACHING

Types of teaching	M	S	GA	GL	GO	GCL	TA	TI	GCA
Hours of face-to-face teaching	12				48				
Horas de Actividad No Presencial del Alumno/a	18				72				

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 %	40 %
Presentations	20 %	40 %
Practical tasks	40 %	80 %

ORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

Evaluation criteria:

(1) Voluntary exercises: 30%
Theoretical exercises: In order to obtain the maximum grade a well-written and reasoned report, with a well-explained approach to the balances corresponding to the proposed system is required.
Practical exercises: In order to obtain the maximum grade the following are required: a checked algorithm that has been validated functionally. Moreover, a report must contain: 1) the approach to the balances corresponding to the proposed system, 2) the required mathematical development to obtain the system model, 3) a flow-chart of the algorithm that explains the resolution strategy, and 4) an analysis of the results obtained by simulation.
The maximum grade of this section is reached by properly carrying out 5 of the 8 proposed exercises.

(2) GUI Exercise: 20%
The evaluation of the GUI will be carried out by the following criteria:
Operability (0-10, weight: 5)
Number of elements (1 point/element, weight: 1)
Number of different elements (1 point/type of element, weight: 3)
Aesthetics (0-10, weight: 2)
Originality (0-10, weight: 2)

(3) Continuous assessment of the subject: 10%
Glossary: each original contribution will be valued at 1 point
Forum:
Question: 1 point
First answer: 2 points
Excellent answer: 3 points
All the points obtained in the glossary and the forum will be summed.
The student will have to obtain 40 points in order to reach the maximum grade of this section.

(4) Final Exam: 40%
The student will have to carry out a complete modelling and simulation of the process in question. All the material available in egela is allowed for its use in the exam.

Final Mark:
A minimum mark of 4/10 is required in each section that is evaluated.

Withdrawal:

The student will have to give advance notice regarding his/her withdrawal from the ordinary call in writing, at least 24 hours before the exam. To do so, he/she will have to send an email to all of the lecturers of the subject in addition to the

coordinator of the Master’s Degree.

EXTRAORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

Evaluation criteria: the same ones as for the ordinary call.

Withdrawal:

The student will have to give advance notice regarding his/her withdrawal from the ordinary call in writing, at least 24 hours before the exam. To do so, he/she will have to send an email to all of the lecturers of the subject in addition to the coordinator of the Master’s Degree.

MANDATORY MATERIALS

Egela virtual classroom
Software: Scilab and Matlab

BIBLIOGRAPHY

Basic bibliography

Ingham, J., Dunn, I.J., Heizle, E., Prenosil, J.E., Snape, J.B. Chemical Engineering Dynamics. An Introduction to Modelling and Computer Simulation. 3rd Ed. Wiley-VCH, 2007
Bird, R.B., Steward, W.E., Lightfoot, E. N., Transport phenomena, 2nd edition, Wiley (2005)

Detailed bibliography

Ramírez, W.F., Computational Methods for Process Simulations, Butterworths, 1989.
Welty, J.R., C.E. Wicks, R.E. Wilson, and G. Rorrer, Fundamentals of Momentum, Heat, and Mass Transfer, 4th edition, Wiley (2000).
Constantinides, A., Mostoufi, N., Numerical Methods for Chemical Engineers with Matlab Applications, Prentice Hall (1999)
Marchand, P., Holland, O.T., Graphics and GUIs with Matlab, 3rd edition, Chapman & Hall/CRC (2003)

Journals

www.sciencedirect.com/science/bookseries/15707946

Web sites of interest

www.scilab.org
www.mathworks.es
cacheme.org
chengineer.com