



## COURSE GUIDE

2024/25

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

**Cycle** .

**Degree** INQUI15b - Master in Chemical Engineering

**Year** .

## COURSE

504253 - Advanced chemical reactors

**Credits, ECTS:** 4,5

## COURSE DESCRIPTION

This course is a continuation of the course Reactor Design of the Bachelor Degree in Chemical Engineering. The knowledge acquired in the design of conventional reactors, as well as new reactors for new processes for Chemical Reaction Engineering, Biochemistry and Electrochemistry is expanded.

The following aspects are addressed: i) fundamentals, analysis and design of reactors for heterogeneous (gas-solid, gas-liquid, liquid-liquid, gas-liquid-solid, solid-solid), electrochemical and biological (with microorganisms and enzymes) processes; ii) reactor selection and optimization of process conditions for catalytic, non-catalytic and multiphase processes; iii) analysis of the current state of technological development and prospects for innovation in the fields of knowledge and industrial implementation; v) analysis of the role of chemical reactors in sustainability and new processes of energy and environmental interest.

The course is closely related to others in the Master's program, such as Modelling and Simulation of Chemical Processes (calculation tools to simulate and design certain configurations of chemical reactors are discussed), as well as with several elective courses describing processes of energy and environmental interest with chemical reactors (such as Refinery and Petrochemical Technologies, Fuels from alternative sources to petroleum, Hydrogen: raw material and energy vector).

## 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.

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.

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.

Manage and supervise all types of facilities, processes, systems and services of the different industrial areas related to chemical engineering.

Design, build and implement methods, processes and facilities for the integrated management of solid, liquid and gaseous supplies and wastes in industries, with the ability to assess their impacts and risks.

### RESULTADOS DE APRENDIZAJE DE LA ASIGNATURA

After completing the course, students will be able to:

- Describe the characteristics of heterogeneous conventional reactors and newly designed reactors.
- Select the most suitable reactor for each process, depending on production, economic, safety, energetic and/or environmental criteria.
- Formulate and handle material and energy conservation equations of reactors.
- Design reactors under real flow conditions by means of flow models.
- Design and optimize the operating conditions of the reactors.

### Theoretical and Practical Contents

1. Introduction: Current state and future prospects in reactor design. Chemical reaction engineering knowledge. New challenges for reactors in the chemical industry: energy, environment, materials. Emerging sectors. Conventional and newly designed heterogeneous reactors.

2. General aspects of catalytic reactors: catalysts, reaction mechanisms and kinetic equations. Consideration of the physical transport stages in the kinetics. Consideration of deactivation. Reactors for kinetic studies. Conventional configurations and new reactors.

3. Fixed bed catalytic reactors: Homogeneous and pseudohomogeneous design models. Considering real flow. Considering deactivation in the design. Strategies for attenuating deactivation.

4. Fluidized bed catalytic reactors: Different fluidization regimes and reactors. Bubbling fluidized bed: fluid dynamics, bed properties, design of the distributor, mixing and segregation indices, flow models for predicting conversion. Pneumatic transport reactors. New reactors.

5. Gas-solid non-catalytic reactors, General aspects: Reactions and kinetic models. Structural and non-structural models. Shrinking core models for particles of constant size: control of different stages. Particles of decreasing size.



6. Gas-solid non-catalytic reactors, Reactor configurations: Fixed and moving beds. Consideration of size distribution. Continuous fluidized bed reactors. Consideration of size distribution and residence time. Reactors for instantaneous reactions. Reactors for new processes of energy and environmental interest.
7. Biphasic reactors (G-L, L-L, S-S), General aspects: Reactions and kinetic modelling. Application of the two-film theory for obtaining kinetic equations in different regimes. Acceleration factor. Transport coefficients. S-S reactions.
8. Biphasic reactors (G-L, L-L, S-S), Reactor configurations: Consideration of flow models. Design of towers for fast reactions. Reactor-settler. Combination of reactors. S-S reactors.
9. G-L-S reactors: Solid reactant in fixed bed (trickle bed). Design for different regimes. Solid reactant in suspension. Comparison of reactors and contact strategies.
10. Electrochemical and nuclear reactors: Energetic and environmental applications. Batch and continuous reactors (stirred tank and plug flow). Combination of reactors. Scale-up solutions. Nuclear reaction engineering.
11. Bioreactors with microorganisms: Kinetics. Structured and unstructured models. Discontinuous and continuous reactors. Mass transfer.
12. Biological reactors with enzymes: Dissolved enzymes. Kinetics. Discontinuous and continuous reactors. Immobilization of enzymes. Reactors with immobilized enzymes.
13. Reactors for the petrochemical industry: FCC unit. Hydroprocessing units. Innovations in the design. Adaptation to new feeds. Challenges and future prospects.
14. Reactors for sustainability: Environmental determining factors. Contribution of reactor design to sustainability. New processes and innovations and future prospects for reactor design.

#### METODOLOGIA (ACTIVIDADES FORMATIVAS)

Actividad Formativa	Hours	Porcentaje presencialidad
Groupwork	9,5	0 %
Case analysis	15	40 %
Expositive classes	23	100 %
Handling sources and resources	25	0 %
Exercises	40	40 %

#### TYPES OF TEACHING

Types of teaching	M	S	GA	GL	GO	GCL	TA	TI	GCA
Hours of face-to-face teaching	17	6	17		5				
Horas de Actividad No Presencial del Alumno/a	25	9	25,5		8				

**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	75 %	85 %
Practical tasks	15 %	25 %

#### ORDINARY EXAMINATION PERIOD: GUIDELINES AND OPTING OUT

3 tasks (non-presential):

1. Written exam (75 %): 2 midterm exams composed of 5/6 theoretical/practical questions. These questions are answered individually, after a period of preparation using available material on e-gela and bibliographic media. If students pass these midterm exams, do not have to do the corresponding parts in the final one.

Assessment criteria: The evaluation of each question will be based on clarity of expression, adequate writing, ability to synthesize and concreteness, as well as originality of the answer (possible internet search for information considered necessary).

Deadlines: The week following completion of the assessed topics in each partial exam (unless agreed to modify the deadline).

2. Individual written work (15 %): A written work on advanced reactor design for a process selected by each student will be carried out. This work will include fundamental aspects of reactor design, of any of the types and for any of the heterogeneous reactions studied in the course or others. The recommended length is around 12 pages (20 pages maximum) including title, nomenclature and bibliography (10 citations maximum).

Assessment criteria: Interest of the reactor studied; Interest of the content of the work from the point of view of reactor design; Concreteness and clarity; Quality and timeliness of the references.

Deadline: The week following the end of the course (unless agreed to modify the deadline).

3. Exercises (10 %): Design exercises of fixed bed and fluidized bed catalytic reactors will be carried out, using in the first case Scilab calculation software. The calculation program will be delivered, as well as the result obtained in the design of each reactor.



Evaluation criteria: Clarity of the calculation program and correctness of the values obtained; adequate description of the resolution procedure(s) used.

Deadline: Before the twelfth week of the course.

Withdrawal: The student will have to give advance notice regarding his/her withdrawal from the ordinary call in writing, at least one week 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**

2 tasks (non-presential):

1. Written exam (80 %): 10 theoretical/practical questions.
  2. Individual written work (10 %): same one as the one described for the ordinary call.
- The assessment criteria are the same as the ones for the ordinary call.

Withdrawal: the same ones as for the ordinary call.

#### **MANDATORY MATERIALS**

- E-gela virtual classroom.
- Scilab Software.

#### **BIBLIOGRAPHY**

##### **Basic bibliography**

- Froment, G.F., Bischoff, K.B., Chemical Reactor Analysis and Design, 2nd Ed, John Wiley, Nueva York, 1990.  
Levenspiel, O., The Chemical Reactor Omnibook, OSU Book Stores Inc., Corvallis, USA , 1996.  
King, M.B., Winterbottom, M., Naumann, E.B., Reactor Design for Chemical Engineers, Blackie Academic & Professional, 1997.  
Coker, A.K., Kayode, C.A., Modeling of Chemical Kinetics and Reactor Design, Elsevier Inc., 2001.

##### **Detailed bibliography**

- Kunii, D., Levenspiel, O., Fluidization Engineering, Butterworth-Heinemann, Newton, USA, 1991.  
Rawlings, J.B., Ekerdt, J., Chemical Reactor Analysis and Design Fundamentals, Nob Hill Publishing, Madison, Wisconsin, 2002.  
Jakobsen, H.A., Chemical Reactor Modeling, Springer Berlin Heidelberg, Berlin, 2008.  
Ranade, V.V., Chaudhari, R.V., Gunjal, P.R., Trickle Bed Reactors, Elsevier B.V., 2011.  
Kunii, D., Chisaki, T., Rotary Reactor Engineering, Elsevier B.V., Amsterdam, 2011.

##### **Journals**

AIChE Journal, Chemical Engineering Education, Chemical Engineering Journal, Chemical Engineering Science, Industrial Engineering Chemistry Research

##### **Web sites of interest**