Proyecto/Guía docente de la asignatura

Subject	DESIGN OF REACTION PROCESSES		
General subject	PROCESS DESIGN		
Module	1. PROCESS AND PRODUCT ENGINEERING		
Degree	MASTER IN CHEMICAL ENGINEERING		
Plan	542	Code	53747
Time period	2º SEMESTRE	Type/Character	MANDATORY
Level/Cycle	MASTER	Course	1º
Credits ECTS	6		
Language	ENGLISH		
Professor/s in charge	JUAN GARCÍA SERNA MARTA RAMOS ANDRÉS		
Department(s)	INGENIERÍA QUÍMICA Y TECNOLOGÍA DEL MEDIO AMBIENTE		
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Fecha de revisión por el Comité de Título	13/07/2026		

1. Situation / Concept of the subject

1.1 Context

Chemical reaction engineering is a core discipline in Chemical Engineering because most industrial processes are ultimately determined by the way chemical transformations are conceived, modelled, controlled and scaled up. The design of reaction processes connects molecular-level phenomena —reaction kinetics, thermodynamics, catalysis and transport limitations— with the practical design of industrial equipment, operating strategies, safety constraints, environmental impact and economic performance.

The subject **Design of Reaction Processes** is conceived as an advanced course within the Master in Chemical Engineering, aimed at consolidating and extending the knowledge acquired in previous studies of chemical reaction engineering. Its main purpose is to enable students to analyse, model and design reaction systems under realistic conditions, including homogeneous and heterogeneous reactions, ideal and non-ideal flow patterns, catalytic systems, multiphase reactors and industrial case studies.

Particular emphasis is placed on the transition from fundamental equations to engineering decision-making. Students will work with reaction models, kinetic data, reactor configurations and process variables in order to select suitable reactor types, estimate conversions and selectivities, evaluate deviations from ideal behaviour and assess the implications of design choices. In this way, the course contributes directly to the development of professional competences required for the conception, design, optimisation and technical evaluation of chemical processes.

The subject also reflects the current evolution of chemical engineering practice, where reactor design is increasingly supported by computational tools, data analysis, simulation, process intensification and sustainability criteria. Therefore, the course combines theoretical foundations with practical problem-solving activities and computer-aided methodologies, preparing students to address complex reaction engineering problems in industrial, research and innovation contexts.

In this context, **Generative Artificial Intelligence tools may be used in selected activities as support for problem solving, especially for programming-related tasks.** Their use may include assistance in structuring numerical algorithms, generating preliminary code, debugging scripts, improving code readability, exploring alternative computational approaches and documenting calculations. However, students will remain responsible for the correct formulation of the engineering problem, the selection of appropriate models and assumptions, the validation of numerical results and the critical interpretation of the solutions obtained. The use of these tools will therefore be understood as a learning and productivity aid, not as a substitute for engineering reasoning or independent academic work.

1.2 Relation with other subjects

This subject is closely related to previous and parallel training in chemical reaction engineering, transport phenomena, thermodynamics, process simulation, process design and chemical technology. In particular, it complements the subject **Process Analysis with Simulators**, since the design of reaction processes provides the kinetic, thermodynamic and reactor modelling basis required for the rigorous simulation and optimisation of complete chemical processes.

1.3 Prerequisites

It is highly recommended that students have previously completed a course in chemical reaction engineering or an equivalent subject during their Bachelor's degree. They should be familiar with basic concepts such as reaction rate, stoichiometry, conversion, selectivity, yield, ideal reactors, material balances and elementary kinetic models.

A solid background in mathematics, chemistry, thermodynamics, transport phenomena and basic process calculations is also advisable. Since the course includes computer-aided problem solving, students are expected to have basic skills in the use of spreadsheets and numerical calculation tools. Previous experience with software such as Python and Microsoft Excel will be useful, although the required computational methodologies will be introduced and applied throughout the course.

2. Competences

2.1 General

CG02. Conceive, project, calculate, and design processes, equipment, industrial facilities and services, in the field of chemical engineering and related industrial sectors, in terms of quality, safety, economy, rational and efficient use of natural resources and conservation of the environment ambient.

CG03. Direct and technically and economically manage projects, facilities, plants, companies and technology centers in the field of chemical engineering and related industrial sectors.

CG04. Carry out the appropriate research, undertake the design and direct the development of engineering solutions, in new or unfamiliar environments, relating creativity, originality, innovation and technology transfer.

CG06. Be able to analyse and synthesize the continuous progress of products, processes, systems and services using criteria of safety, economic viability, quality and environmental management.

CG07. Integrate knowledge and face the complexity of making judgments and decision making, based on incomplete or limited information, including reflections on the social and ethical responsibilities of professional practice.

CG10. Adapt to changes, being able to apply new and advanced technologies and other relevant developments, with initiative and entrepreneurial spirit.

CG11. Possess the skills of autonomous learning to maintain and improve the skills of chemical engineering that allow the continuous development of the profession.

2.2 Specific

CEP01. 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.

CEP02. Design products, processes, systems and services of the chemical industry, as well as the optimization of others already developed, taking as a technological base the various areas of chemical engineering, comprehensive processes and transport phenomena, separation operations and engineering reactions chemical, nuclear, electrochemical and biochemical.

CEP04. Have the ability to solve problems that are unfamiliar, incompletely defined, and have competing specifications, considering the possible solution methods, including the most innovative ones, selecting the most appropriate one, and being able to correct the implementation, evaluating the different design solutions .

CEP05. Direct and supervise all types of facilities, processes, systems and services of the different industrial areas related to chemical engineering.

3. Objectives

The general objectives are:

- Select the type of reactor and the most appropriate operating conditions based on the chemical transformation process.
- Apply calculation models to quantify conversions and equipment sizing in homogeneous and heterogeneous reactors.
- Analyze the influence of deviations of flow ideality on the behavior of reaction systems.

Specific objectives are:

- Analysis of processes with chemical reaction. Fundamental calculus equations. Reaction systems and flow models.
- Complex reactions. Types. Differential and global selectivity. Optimization of reactor configurations.
- Heterogeneous Reactors. Fixed Bed Catalytic Reactor: simple and complex calculation models. Fluidized Bed Catalytic Reactor. Three-phase reactors: trickle-bed reactor and slurry reactor. Calculation methods.
- Applications of non-ideal flow in Chemical Reaction. Macromixing approximation. Simple and combined models. Micromixing.

4. Contents and/or thematic blocks

Block 1: DESIGN OF CHEMICAL REACTION

Carga de trabajo en créditos ECTS: 6

a. Context and justification

See 1.

b. Learning objectives

See 3.

c. Contents

The subject is developed in English language mainly.

The contents are divided into 5 topics:

Topic 1. Introduction to Chemical Reaction Engineering

Reaction overview. Radiography of the chemical sector. Conversion, extent, selectivity and yield. Reaction matrix for multiple reactions. Thermodynamics, chemical equilibrium and equilibrium conversion.

Topic 2. Data driven and machine-learning kinetics

Kinetic estimation as supervised learning (loss, validation, regularisation). White-box / grey-box / black-box models. Data-driven rate-law discovery and hybrid models. Physical constraints and responsible use.

Topic 3. Kinetics of homogeneous reactions

Rate of reaction. Reaction matrix. Multiple chemical reactions: series and parallel networks. Temperature dependence. Kinetic fit: derivative, integral and general simulation methodology. Objective function. Parameter identifiability and error. Computer-aided solutions. Examples.

Topic 4. Homogeneous catalysis

Concept of catalysis. Catalytic cycle. Turnover number and frequency. Acid-base catalysis. Organometallic and transition-metal catalysis. Industrial catalytic cycles. Biocatalysis and enzyme kinetics: Michaelis-Menten and inhibition. Kinetics of homogeneously catalysed reactions.

Topic 5. Heterogeneous catalysis: fundamentals and kinetics

Definitions. Catalyst composition: active phase, support and promoters. Texture and basic characterisation. Adsorption and isotherms. Surface reaction mechanisms: Langmuir-Hinshelwood-Hougen-Watson, Eley-Rideal and Mars-van Krevelen. Formal kinetic models. Derivation and discrimination of rate equations.

Topic 6. Catalyst deactivation

Deactivation mechanisms: poisoning, fouling and coking, sintering, leaching. Deactivation kinetics and activity decay laws. Effect on reactor operation. Temperature compensation and regeneration. Reactor selection for deactivating catalysts.

Topic 7. Transport and reaction in catalytic systems

External mass and heat transfer. Internal diffusion. Thiele modulus and effectiveness factor. Combined resistances. Weisz-Prater criterion. Apparent kinetics and activation energy. Non-isothermal catalyst pellet.

Topic 8. Ideal reactors and energy balances

Batch reactor. Plug flow. Continuous stirred tank. Main equations. Reactor combinations and recycle. Energy balances: adiabatic and non-adiabatic operation. Multiple steady states and stability. Thermal runaway and parametric sensitivity. Optimal temperature progression. Selectivity optimisation.

Topic 9. Non-ideal Flow

Age functions. RTD. Moment analysis. RTD from tracers. Basic models: dispersion and tanks-in-series. Combined and compartment models. Convolution. Macromixing. Micromixing. Segregation.

Topic 10. Heterogeneous and multiphase reactors

Packed bed: pseudo-homogeneous and heterogeneous models. Hot spots. Fluidised bed. Gas-solid non-catalytic: shrinking-core model. Gas-liquid reactors: enhancement factor and Hatta number. Multiphase reactors. Trickle bed and slurry reactors. Selection and scale-up. Case studies.

d. Teaching methods

See 5.

e. Working plan

Week 6:	Assignment 1 (Task #1) – Kinetic determination
Week 9:	Assignment 2 (Task #2) – Multiphase Reactor case study
Week 12:	Assignment 3 (Task #3) – Lab example analysis
Week 15:	Assignment 4 (Task #4) – Modelling of a reactor

f. Evaluation

See 7.

g Material docente

Esta sección será utilizada por la Biblioteca para etiquetar la bibliografía recomendada de la asignatura (curso) en la plataforma Leganto, integrada en el catálogo Almena y a la que tendrán acceso todos los profesores y estudiantes. Es fundamental que las referencias suministradas este curso estén actualizadas y sean completas. Los profesores tendrán acceso, en breve, a la plataforma Leganto para actualizar su bibliografía recomienda ("Listas de Lecturas") de forma que en futuras guías solamente tendrán que poner el enlace permanente a Leganto, el cual también se puede poner en el Campus Virtual.

g.1 Bibliografía básica

The reference book available in the electronic library of UVa will be:

- Coulson and Richardson's chemical engineering. Volume 3A, Chemical and biochemical reactors and reaction engineering e-book UVa
- Engineering of Chemical Reactions, O. Levenspiel.
- Elements of Chemical Reaction Engineering, Scott Fogler.
- Heterogeneous Catalysis in practice. Charles N. Satterfield

- Chemical Engineering Kinetics, J.M. Smith
- Chemical Reaction Engineering Handbook of Solved Problems, Stanley M. Walas.

g.2 Bibliografía complementaria

g.3 Otros recursos telemáticos (píldoras de conocimiento, blogs, videos, revistas digitales, cursos masivos (MOOC), ...)

Included in Campus Virtual.

h. Recursos necesarios

Python and Excel MATLAB

Microsoft Teams.

i. Temporalización

Topic 1. Introduction to Chemical Reaction Engineering (4 h)
Topic 2. Data driven and machine-learning kinetics (3 h)
Topic 3. Kinetics of homogeneous reactions (9 h)
Topic 4. Homogeneous catalysis (4 h)
Topic 5. Heterogeneous catalysis: fundamentals and kinetics (7 h)
Topic 6. Catalyst deactivation (3 h)
Topic 7. Transport and reaction in catalytic systems (4 h)
Topic 8. Ideal reactors and energy balances (9 h)
Topic 9. Non-ideal flow (6 h)
Topic 10. Heterogeneous and multiphase reactors (9 h)

5. Teaching methods and methodological principles

The subject is eminently practical oriented to help the students in solving reaction problems using computer aided solutions.

Part of the subject will be complemented with a FLIPPED CLASSROOM in few cases, where the students will receive material and can interact with different questionaries. Professors will analyse this material to focus the class in the most difficult parts identified.

a. Face-To-Face Activities (in class)

j1. Master Classes

Throughout the theoretical classes the contents are developed taking into account the skills and abilities that the student should acquire.

The classes are presented using PowerPoint or Keynote presentations that the students have previously available to download from the subject's website in the Campus Virtual.

Student participation is encouraged at all times during the class.

j2. Practical classes

The practical classes in the computer target the student to learn and acquire capabilities with different tools important to solve reaction engineering problems.

A number of real laboratory and industrial case studies will be analysed.

j3. Face-to-face tutorials on-line assignment

The students can raise the doubts in the preparation of the tasks or any other question they might have.

To encourage the use of the tutorials an on-line Excel file is used, shared by all students and teachers. Each week the teacher indicates the free tutoring "slots" and the students sign up.

j4. Final exam

Students will take a final exam in the computer.

j5. Partial evaluations

Some partial evaluation may be carried out to check the degree of learning by favouring continuous assessment.

b. Non Face-to-Face Activities (at home or somewhere else)

k1. Tasks

The students will develop the kinetic or reaction tasks in the computer.

k2. Virtual contact with the teacher

Using the Campus Virtual, e-mail, LinkedIn or any other means.

k3. Virtual aula

All the content of the course is available in the Campus Virtual UVa:

http://campusvirtual.uva.es

k4. Flipped material classroom

All the flipped material and questionaries will be available on the Campus Virtual UVa:

http://campusvirtual.uva.es

Microsoft Forms may also be used.

6. Dedicational time of the student to the subject

PRESENTIAL ACTIVITIES	HORAS	NON PRESENTIAL ACTIVITIES	HOURS
Theory	30	Tasks 1+2+3+4	60
Practice in the aula	28	Study and autonomous work individual (and flipped material if any)	30
Seminars	0		
Laboratories	0		
Tutorial service			
Evaluation (out of the official examination period)	2		
Total face-to-face activities	60	Total non face-to-face activities	90

7. System and characteristics of the evaluation

<table>
<tr><th>INSTRUMENT/ PROCEDURE</th><th>VALUE IN FINAL MARK (%)</th><th>REMARKS</th></tr>
<tr><td>TEST</td><td>30%</td><td>WRITTEN</td></tr>
<tr><td rowspan="4">TASKS</td><td>15%</td><td>Task #1</td></tr>
<tr><td>15%</td><td>Task #2</td></tr>
<tr><td>5%</td><td>Task #3</td></tr>
<tr><td>20%</td><td>Task #4</td></tr>
<tr><td rowspan="2">ATTITUDE IN CLASS</td><td>10%</td><td>PARTICIPATION
It will be considered: participation in class, generation of ideas, attitude and relation with the other classmates and use of the class main/optional materials.</td></tr>
<tr><td>5%</td><td>FLIPPED CLASSROOM
It will also be specifically considered the work and responses on the flipped material if any (if not this will be included in the participation)</td></tr>
<tr><th colspan="3">MARK CRITERIA</th></tr>
<tr><td colspan="3">

- Ordinary call:
  - As per specification in the table.
- Extraordinary call:
  - A minimum mark of 4.0 is required in the written test (exam) to pass.
  - The available assignments marks and attitude in class marks will be preserved to calculate the final mark. The final mark will consider:
    - Task 1-4 *(39.3%)*
    - Attitude in class *(10.7%)*
    - Extraordinary written test (examination) *(50%)*
- Extraordinary final-year examination session (Convocatoria extraordinaria Fin de Carrera, Article 35 of the UVa Academic Regulations ROA), given the nature of the course, students shall be assessed individually through a written examination covering the course contents (100%). This assessment shall ensure the acquisition of the same competences and learning outcomes set out in this course guide.

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8. Final remarks

USE OF GENERATIVE ARTIFICIAL INTELLIGENCE

The use of Generative Artificial Intelligence is permitted for certain tasks and activities in this course.

- To determine which tasks allow its use, it is advisable to review the specifications of said tasks in detail when they appear in the virtual classroom, in the course schedule, and/or in the detailed syllabus, and/or by consulting directly with the course instructors.
- It is the student's responsibility to know and apply these specific requirements.

Furthermore, it is recommended to consider the general and ethical recommendations of the University of Valladolid for the use of this technology:

https://digital.uva.es/uso-de-la-ia-generativa-en-docencia/