

## **COURSE DATA**

Data Subject		
Code	34760	
Name	Chemical reaction engineering I	
Cycle	Grade	
ECTS Credits	6.0	
Academic year	2022 - 2023	

Study (s)		
Degree	Center	Acad. Period
		year
1401 - Degree in Chemical Engineering	School of Engineering	2 Second term

Subject-matter					
Degree	Subject-matter	Character			
1401 - Degree in Chemical Engineering	16 - Chemical reaction engineering	Obligatory			

#### Coordination

Name	Department
CHAFER ORTEGA, AMPARO	245 - Chemical Engineering
SAN VALERO TORNERO, PAU	245 - Chemical Engineering

## SUMMARY

Chemical Reaction Engineering I is a part of the matter of the same name. His general objective is the increase of the knowledge of kinetics of chemical reactions and the combination of this knowledge with the bases of chemical engineering in order to apply them to the design and operation of the reactors of the chemical and biochemical industry. It is a compulsory subject that is imparted in the second semester of the second year of the Chemical Engineering degree. It has assigned 6 ECTS credits.

With this subject of study we tries to give an overview of the Chemical Reaction Engineering and to provide the students the necessary knowledge of the basics of the processes of chemical reaction, introducing the necessary tools for analysis and design of chemical reactors. These tools will be the combination of balances with the rate equations. This way, it will be established the essential bases in order to a successfully application. Once the items will be introduced they will be used in order to solve a series of problems. Students will practice with these concepts and procedures in other subject.



The content of this subject is: Kinetics of chemical reactions. Ideal reactors. Basic equations of design. Design of ideal reactors. Biochemical reactors, polymerization reactors, membrane reactors. Basis of Biochemical Engineering.

The theory classes will be taught in Valencian and the practical sessions as stated in the assignment form on the web of the degree.

## **PREVIOUS KNOWLEDGE**

#### Relationship to other subjects of the same degree

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

#### Other requirements

Differential and integral calculation, systems of equations solution (algebraic and differentials), numerical calculation, optimization, statistics, coordinate systems.

Stoichiometry, kinetics.

Equilibrium and heat of reaction, transmission of heat.

Change of units, Mass, energy and momentum balances, mass and heat transfer, mechanics of fluids.

Economy: Basic slight knowledge.

Software: Basic programs, programs to solve systems of equations (Polymath, MATLAB, etc).

#### **OUTCOMES**

#### 1401 - Degree in Chemical Engineering

- G3 Knowledge of basic and technological subjects that allows students to learn new methods and theories and provides them with versatility to adapt to new situations.
- G4 Ability to solve problems with initiative, decision-making skills, creativity and critical reasoning and to communicate and transmit knowledge, abilities and skills in the field of industrial engineering.
- G5 Knowledge to carry out measurements, calculations, assessments, appraisals, surveys, studies, reports, work plans and analogous work.
- G6 Ability to deal with specifications, regulations and mandatory standards.
- G10 Ability to work in a multilingual and multidisciplinary environment.
- G11 Knowledge, understanding and ability to apply the necessary legislation for practising professionally as a qualified industrial technical engineer.
- TE1 Knowledge of material and energy balances, biotechnology, matter transfer, separation operations, chemical reaction engineering, reactor design, and valorisation and transformation of raw materials and energy resources.



- TE2 - Ability to analyse, design, undertake simulations and optimise processes and products.

## **LEARNING OUTCOMES**

#### Learning results.

- To know and understand the basics of the applied kinetic chemistry. (G3,TE1)
- To apply the principles of mass and energy conservation in systems with chemical reaction. (G4,TE1,TE2)
- To apply the principles of thermodynamics and kinetics in systems with chemical reactions. (G4)
- To know the characteristics and mathematical models to describe the ideal reactors. (G3)
- To analyse the operation and dimensioning of the ideal isothermal reactors. (G3,G5,G6)
- To select the type and number of reactors to attain a conversion value. (G4)
- To know the specificities and applications of various types of industrial reactors: Catalytic, biochemical, of polymerization, of membrane. (G5)
- To know and apply the safety principles related to chemical reactors. (G6,G11)
- To prepare written reports. (G5,G10)
- To prepare designs both in individual and in group way. (G4)

### At the end of the course students should be able to:

- To understand the phenomena involved in chemical reactions. To know the nomenclature and terminology.
- To calculate the composition changes and their impact on the reaction rate.
- To understand the parameters that influence the reaction rate and how this influence is.
- To combine aspects of the kinetics with which characterize the behaviour of the reactor (continuous, batch, etc.).
- To apply mass and energy balances necessary for the design and analysis of ideal reactors. This
- includes cases of varying density and multiple reactions, as well as membrane reactors and biochemical reactors.
- Apply this knowledge to design and prediction of reactor operation.
- To understand how the different chemical reactors work and to be able to make recommendations for different cases.
- Understand the special features of reactors such as the polymerization ones.
- To implement calculating procedures in a reasonable manner, justifying the results.
- To recognize the different kinds of information that appear in text associated with chemical reactions and reactors.
- To collect the information needed to formulate and solve a problem related to the design and/or analysis of a reactor.
- To manage the information with criteria.
- To identify and explain the physical meaning of each of the terms of the balance equations.
- To describe the equations of the chemical reactions kinetic and heat transfer.
- To explain the distinguishing features of the different ideal reactors.



Besides during the course will promote the acquisition by students of other social and technical abilities such as to:

- To extract information from the statement of a problem.
- To interpret and translate as variables the data of a problem.
- To interpret correctly other data, definitions and relationships of the process and write them in form of equations.
- To write the appropriate boundary conditions for the integration and resolution of problems.
- To solve the problem using appropriate mathematical tools.
- To interpret and reasoning the results of a problem.
- To interpret experimental results and report them.
- To organize calculations in a systematic way
- To make calculations accurately and substantiated.
- · Capacity for analysis and synthesis.
- · Trained to work individually and in groups
- Ability to allocate time between tasks effectively.
- Ability to argue with logic and reasoned criteria.

## **DESCRIPTION OF CONTENTS**

#### 1. INTRODUCTION AND GENERAL CONCEPTS.

Chemical engineering and chemical reactors engineering. The Chemical Reactors Engineering on Industry. Examples.

#### 2. PHENOMENOLOGY OF CHEMICAL REACTIONS.

Stoichiometry. Chemical schemes simple, global, multiples. Composition measures. Static and dynamic systems. Simple and multiple reactions. Measures of the progress of the reaction, selectivity, etc. Chemical equilibrium. Chemical Kinetics.

#### 3. IDEAL REACTORS. ISOTHERMAL BEHAVIOR.

Introduction to design of chemical reactors. The Continuous Stirred Tank Reactor (CSTR). The discontinuous stirred tank reactor (batch). The continuous tubular or plug flow reactor (PFR). Semicontinuous reactors. Changing heat systems for isotherm behaviour. Combination of reactors

#### 4. SELECCTION AND EXTENSIONS OF REACTORS

Combination of reactors: graphic o analytical procedures of design. Reactors of plug flow (RFP) with recirculation. Selection of best design alternative: simple reactor or combination .



### 5. MULTIPLE REACTIONS.

Qualitative and quantitative analysis of different systems. Optimization. Polymerization Reactors.

#### 6. BIOCHEMICAL REACTORS.

Introduction to biochemical engineering. Enzyme and microbial kinetics. Design of biochemical reactors.

## WORKLOAD

Hours	% To be attended
35,00	100
25,00	100
20,00	0
5,00	0
15,00	0
15,00	0
30,00	0
5,00	0
L 150,00	
	35,00 25,00 20,00 5,00 15,00 15,00 30,00 5,00

## TEACHING METHODOLOGY

1 .- Lessons in the classroom. (G3,G4,G5,G6,G10,G11,TE1,TE2)

These lectures will be of theory or problems according to the needs of the moment. Thus, first it will be presented the theory and then the practical applications. The model used is as follows: the theory will be exposed briefly by the teacher.

Practical classes of problems will be developed following two models. In some of the lectures the teacher will solve a series of sample problems for to identify the essential elements of the approach and problem resolution. In other kinds of problems will follow a participatory model following a seminar methodology, students will solve problems individually or arranged in groups (cooperative learning), under the supervision of the teacher. After the work, the problems will be collected, analysed and corrected by the teacher or the students themselves.

2 .- Seminars. (G3,G4,G5,G6,G10,G11,TE1,TE2)

Students solve problems in group, using informatic tools.



## **EVALUATION**

The final grade will have two contributions, the first one (70 %) corresponds to the exam (G3,G4,G5,G6,G10,G11,TE1,TE2), the second one (30 %) (G3,G4,G5,G6,G10,G11,TE1,TE2) will be related to continuous evaluation with activities in the classroom along the course (20 %) and with the student resolution of test at virtual classroom (10 %). If the continuous evaluation goes down the student qualification, the mark will be calculated only with the results of exam.

The exam will consist of theory (questions) and problems, for answer the theory the students can dispose of a form (one sheet), and for the problems solution they can use books, notes..., but without solved problems.

Examination and activities will be scored over 10 points; to pass the subject should at least get 4.0 points in the exam and 5.0 in the final grade.

The only recoverable activity is the examination, in the second call

In any case, the assessment system will be governed by that established in the Reglament de Avaluació i Qualificació de la Universitat de València per a títols de Grau i Màster (<a href="http://links.uv.es/7S40pjF">http://links.uv.es/7S40pjF</a>)

## **REFERENCES**

#### **Basic**

- BERNA. A., CHÁFER, A. i ROSSELLÓ, C. Enginyeria dels Reactors Químics. Problemes i qüestions. Universitat de València. 2009. ebook en UV
- ESCARDINO, A. i BERNA. A. Introducció a l'Enginyeria dels Reactors Químics. Universitat de València, 2003. ebook en UV
- FOGLER, H. S. "Elements of Chemical Reaction Engineering", 3rd ed., Prentice Hall. New Jersey, 1999. Hi ha una edició en castellà: Elementos de Ingeniería de las Reaccciones Químicas Prenctice Hall, México 2001.

#### Additional

- CUTLIP, M.B. i SHACHAM, M. Problem solving in Chemical Engineering with numerical methods Prentice Hall 1999.
- LEVENSPIEL, O. "The Chemical Reactor Omnibook". Ed. Oregón State University. 1993. Traduït per Editorial Reverté. Barcelona. 1986
- SANTAMARÍA, J.M.; HERGUIDO, J.; MENÉNDEZ, M.Á. i MONZÓN, A. Ingeniería de reactores, Síntesis, Madrid 1999.