COURSE DATA

Data Subject	
Code	34761
Name	Chemical reaction engineering II
Cycle	Grade
ECTS Credits	6.0
Academic year	2023 - 2024

Study (s)

Degree	Center	Acad. year	Period
1401 - Degree in Chemical Engineering	School of Engineering	3	First term

Subject-matter

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

Coordination

Name	Department
CERISUELO FERRIOLS, JOSEP PASQUAL	245 - Chemical Engineering
IZQUIERDO SANCHIS, MARTA	245 - Chemical Engineering

SUMMARY

Chemical Reaction Engineering II 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.

Chemical reactors are the object of study of the Chemical Reaction Engineering. This study has two slopes, the analysis of the behaviour and the design of the equipment and of its operating. It is a very applied field. With this knowledge one can study the behaviour and the design of different chemical reactors.

The practical part tries of study different applications of the exposed concepts, thus, for example, the necessary volume of the reactor to get a conversion or a production will be calculated, and it will be analysed the effect of modify some parameter, as for example the temperature of operation. The interpretation of results will be an important part of the learning process.

It is a compulsory subject that is imparted in the first semester of the third 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: Non-isothermal reactors. Non-ideal reactors. Heterogeneous reactors. Catalytic reactors. Safety and chemical reactors.

Remarks: Classes of both theory and problems will be taught in Valencian as it appears in the subject sheet available 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

It would be convenient to have the following prior knowledge:
To have taken the subject Chemical Reaction Engineering I.
Differential and integral calculus, solution of systems of equations (algebraic and differential), numerical methods, optimization, coordinate systems.
Stoichiometry, kinetics.
Equilibrium and heat of reaction.
Mass and energy balances, heat and matter transfer, fluid mechanics.
Specialized software: Polymath, MATLAB

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 and non-isothermal reactors. (G3, G5, G6)

• To select the type and number of reactors to attain a conversion value. (G4)

• To understand the deviations of the ideal flow. (G5, TE1)

• 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)

Skills to acquire

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. (G3, G10, TE1)

• To calculate the composition changes and their impact on the reaction rate. (G4)

• To understand the parameters that influence the reaction rate and how this influence is. (G4, G5)

• To combine aspects of the kinetics with which characterize the behaviour of the reactor (continuous, batch, etc.). (G5, G6)

• To combine aspects of the kinetics of chemical reaction with the mass transfer for heterogeneous reactions. (G3, G4)

• To apply mass and energy balances necessary for the design and analysis of ideal reactors. (G3, G4)

• Apply this knowledge to design and prediction of reactor operation. (G3, G4, TE2)

• To understand how the different chemical reactors work and to be able to make recommendations for different cases. (G4, G5, G11, TE2)

• To implement calculating procedures in a reasonable manner, justifying the results. (G4, G5, G11, TE2)

Besides during the course will promote the acquisition by students of several **social and technical skills**, including the following:

• To recognize the different kinds of information that appear in text associated with chemical reactions and reactors. (G3, G10)

• To collect the information needed to formulate and solve a problem related to the design and/or analysis of a reactor. (G3, G4)

• To manage the information with criteria. (G4, G5)

• To identify and explain the physical meaning of each of the terms of the balance equations. (G3, G4)

• To describe the equations of the chemical reactions kinetic and heat transfer. (G3, G4)

• To explain the distinguishing features of the different ideal reactors. (G3, G4)

• To extract information from the statement of a problem. (G4, G5)

• To interpret and translate as variables the data of a problem. (G4, G5)

• To interpret correctly other data, definitions and relationships of the process and write them in form of equations. (G4, G5)

• To write the appropriate boundary conditions for the integration and resolution of problems. (G4, G5)

• To solve the problem using appropriate mathematical tools. (G4, G5)

• To interpret and reasoning the results of a problem. (TE2)

• To interpret experimental results and report them. (G3, G5, TE2)

• To organize calculations in a systematic way (G3, G5, TE2)

• To make calculations accurately and substantiated. (G4)

• Capacity for analysis and synthesis. (TE1, TE2)

• Trained to work individually and in groups (G4, G10)

• Ability to allocate time between tasks effectively. (G4, G10)

• Ability to argue with logic and reasoned criteria. (G4, G10)

• To write reports of issues solved in a way that reveals the information used, the procedures and analysis of results (TE1, TE2)

• To show in public the results with use of a convenient means (G10, G11)

DESCRIPTION OF CONTENTS

1. Ideal reactors. Non-isothermal reactors.

The continuous stirred tank reactor (CSTR). The batch reactor. The plug flow reactor (PFR). Semicontinuous reactor. Series of reactors. Multiple reactions.

2. Stability of the chemical reactor behaviour.

Steady state multiplicity. Control problems in the chemical reactors.

3. Non-ideal flow in chemical reactors.

The distribution of residence times function (RTD). Reactor modelling with the RTD. Conversion levels in non-ideal reactors.

4. Heterogeneous reactors.

Transport processes in solid-fluid heterogeneous reactions. Models for solid-fluid reactions. Determination of limiting step.

5. Catalytic reactors.

Catalytic reactions kinetic. Design application.

6. Safety and chemical reactors.

Explosions. Overpressure. Design of safer reactors.

7. Non-conventional reactors

CVD reactors. Membrane reactors. Supercritical reactors.

WORKLOAD

ACTIVITY	Hours	% To be attended
Classroom practices	35,00	100
Theory classes	25,00	100
Readings supplementary material	10,00	0
Preparation of evaluation activities	50,00	0
Preparing lectures	12,00	0
Preparation of practical classes and problem	17,00	0
Resolution of online questionnaires	1,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

To successfully develop the subject, different strategies must be followed: theoretical lessons and solving-problem lessons, autonomous work and participation in tutorials.

Classroom lessons (G3, G4, G5, G6, G10, G11, TE1, TE2)

In these classes the theoretical contents of the subject are taught and problems are solved according to the needs of each moment. In the first place, the theoretical contents are presented in a participatory master class format, pointing out the texts in which the subject can be found, promoting autonomous work, to later solve a series of standard problems by lecturers in practical classes, so that students learn to identify the essential elements of solving the problem. The materials used in the theoretical classes and the collection of problems (with class problems and to be solved at home) will be shared through the Virtual Classroom.

Throughout the semester, the resolution and delivery of various problems individually or in small groups is also proposed for correction and qualification, and this qualification will be part of the final evaluation of the subject.

Autonomous study and work. (G3, G4, G5, G6, G10, G11, TE1, TE2)

The students will have to study on their own, to assimilate the exposed knowledge, and practice them with the proposed problems. Some of the proposed problems will not be solved in class so that students can prepare them and solve doubts attending the tutorial sessions.

Tutorials. (G3, G4, G5, G6, G10, G11, TE1, TE2)

Students will be able to consult the lecturers either directly in class or by attending the tutorials at the established time or through the Virtual Classroom tutoring forum.

EVALUATION

The assessment of student learning will be based on the activities of the course (questionnaires and problems delivered) and the examination(s).

Regarding the examination(s), students can choose one of the following options in the first call:

(1) Single final examination on an official date where the entire content of the course will be evaluated.

(2) Partial examination on a date indicated at the beginning of the course and a second partial examination on an official date. Thus, the overall mark of the examinations will be calculated as the weighted average of the two partial examinations.

In the second call, the examination will be based only on option (1), that is, a single final examination in the official date where the entire content of the course will be evaluated.

The final grade will be obtained as the highest of:

• the weighting between the average mark of the questionnaires (15%), problems delivered (15%) and the mark of the exam(s) (70%), or

• The mark of the knowledge exam(s) plus 5% of the weighted average mark of the activities (questionnaires and problems delivered).

If the examination mark is less than 4.5 out of 10, the final mark will be the one obtained in the examination.

The course will be considered as passed when the mark obtained is equal to or greater than 5 out of 10.

In any case, the evaluation system will be governed by the one established in the Regulation of Evaluation and Qualification of the University of Valencia for Degrees and Masters (https://goo.gl/uddys2).

REFERENCES

Basic

- ESCARDINO, A. i BERNA. A. Introducció a l'Enginyeria dels Reactors Químics. Universitat de València, 2003. (e-book en la biblioteca UV)
- BERNA. A., CHÁFER, A. i ROSSELLÓ, C. Enginyeria dels Reactors Químics. Problemes i qüestions. Universitat de València. 2009 (e-book en la biblioteca UV)
- FOGLER, H. S. "Elements of Chemical Reaction Engineering", 7th ed., Prentice Hall. New Jersey, 2020.
  http://umich.edu/~elements/5e/index.html

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.
- METCALFE, I. S. Chemical Reaction Engineering. A First Course. Oxford University Press. Oxford 1997.
- SANTAMARÍA, J.M.; HERGUIDO, J.; MENÉNDEZ, M.Á. i MONZÓN, A. Ingeniería de reactores, Síntesis, Madrid 1999.
- CONESA, J. i FONT, R. Reactores heterogéneos. Universitat dAlacant. 2001

- GONZÁLEZ VELASCO, J.R. i altres Cinética química aplicada, Síntesis, Madrid (1999)
- IZQUIERDO, J.F., CUNILL, F., TEJERO, J., IBORRA, M. i FITÉ, C. Cinética de las reacciones químicas. Edicions de la Universitat de Barcelona, sèrie Metodologia número 16, 2004.