

Course guide

320065 - ERQ - Chemical Reaction Engineering

Last modified: 19/04/2023

Unit in charge: Terrassa School of Industrial, Aerospace and Audiovisual Engineering
Teaching unit: 713 - EQ - Department of Chemical Engineering.

Degree: BACHELOR'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Compulsory subject).

Academic year: 2023 **ECTS Credits:** 6.0 **Languages:** Catalan, Spanish

LECTURER

Coordinating lecturer: MANUEL JOSE LIS ARIAS

Others:

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:

5. CHE: Knowledge of material and energy balances, biotechnology, the transfer of materials, separation operations, chemical reaction engineering, the design of reactors, and the reuse and transformation of raw materials and energy resources.

Transversal:

2. SELF-DIRECTED LEARNING - Level 3. Applying the knowledge gained in completing a task according to its relevance and importance. Deciding how to carry out a task, the amount of time to be devoted to it and the most suitable information sources.
3. TEAMWORK - Level 3. Managing and making work groups effective. Resolving possible conflicts, valuing working with others, assessing the effectiveness of a team and presenting the final results.
4. EFFECTIVE USE OF INFORMATION RESOURCES - Level 3. Planning and using the information necessary for an academic assignment (a final thesis, for example) based on a critical appraisal of the information resources used.

TEACHING METHODOLOGY

- Face-to-face lecture sessions.
- Face-to-face practical work sessions.
- Independent learning and the resolution of case studies.
- Group learning and the completion of a project.

In the face-to-face lecture sessions, the lecturer will introduce the basic theory, concepts, methods and results for the subject and use examples to facilitate students' understanding.

Practical class work will be covered in three types of sessions:

a) Sessions in which the lecturer will provide students with guidelines on how to analyse processes and solve problems using simple calculus and problem solving software (70%).

b) Sessions in which the flowcharts students have compiled in groups will be discussed (8%).

c) Examination sessions (12%).

d) Directed-activity seminars, in which students are divided into work groups. At the beginning of the year, each group will be assigned a project to work on and present orally at the end of the semester. The lecturer will hold monitoring sessions with each group (10%).

Students will be expected to study in their own time so that they are familiar with concepts and are able to solve the exercises set, whether manually or with the help of a computer.

LEARNING OBJECTIVES OF THE SUBJECT

In this subject, students will learn to extrapolate experimental data from the laboratory to the production scale (a skill used regularly by chemical engineers working in industry).

Students will carry out various industrial chemical reactions in chemical reactors; virtually all of the reactions will have peculiarities that require a different type of reactor to be used.

Students will learn which criteria should be applied in reactor design on the basis of the type of reaction: homogeneous, heterogeneous, single, complex or autocatalytic. Within the group of catalytic reactions, students will study the special cases of microbial and enzyme kinetics.

Students will consider not only production-related aspects but also environmental concerns: setting up chemical reactors to ensure minimal waste, achieving optimal energy use, and minimising environmental impact.

On completing the subject, students will be able to design a real reactor, including selecting a stationary or non-stationary model for the reaction system and determining a reaction's energy and catalyst needs.

STUDY LOAD

Type	Hours	Percentage
Hours medium group	30,0	20.00
Self study	90,0	60.00
Hours large group	30,0	20.00

Total learning time: 150 h

CONTENTS

TOPIC 1: RATE LAWS AND STOICHIOMETRY

Description:

- Review of chemical kinetics.
- Orders of reaction.
- Analysis of reaction rate data.
- Assessment of laboratory reactors.
- Single and multiple reaction systems.
- Reaction systems with chemical equilibrium.
- Microbial and enzyme kinetics.
- Using experimental data to define reactor parameters: batch case.

Specific objectives:

On completing this topic, students will be able to:

- Review concepts such as order of reaction and molecularity from a reactor-oriented viewpoint.
- Interpret data obtained in a laboratory reactor.
- Understand various chemical reactions in the form of examples and their influence on reactor parameters.
- Identify the differences between chemical and biological systems from a kinetic standpoint.
- Identify the relationships between the stoichiometry of chemical reactions, both with and without equilibrium, and kinetic profiles.
- Apply balances to reactors with multiple-reaction systems.

Full-or-part-time: 15h

Theory classes: 4h

Laboratory classes: 1h

Self study : 10h

TOPIC 2: IDEAL ISOTHERMAL REACTORS

Description:

- Design equations for simple isothermal reactions.
- Batch reactors and stationary reactors.
- Design of CSTRs and PFRs.
- Advantages and disadvantages.
- Loss of pressure in reactors.

Specific objectives:

On completing this topic, students will be able to:

- Choose a system to represent a chemical reaction according to the work method used.
- Define balance variables and extrapolate them to the reactor scale.
- Understand the various types of reactors and their design equations.
- Understand the influence of compositional changes inside the reactor according to the work method used.
- Calculate residence time for each type of reactor.

Full-or-part-time: 25h

Theory classes: 10h

Laboratory classes: 5h

Self study : 10h

TOPIC 3: NON-ISOTHERMAL REACTOR DESIGN

Description:

- Non-isothermal batch reactors.
- Non-isothermal continuous-flow reactors.
- Conversions to equilibrium.
- Non-adiabatic reactor operations.
- Multiplicity of steady states: ignition and extinction in reactors.

Specific objectives:

On completing this topic, students will be able to:

- Apply energy balances in chemical reactors according to the work method used.
- Assess the energy needs of a chemical reactor, according to the reaction.
- Understand chemical equilibrium systems and system temperature.
- Understand the heating and cooling of chemical reactors: jackets and interior coils.

Full-or-part-time: 23h

Theory classes: 11h

Laboratory classes: 2h

Self study : 10h

TOPIC 4: CATALYSIS AND CATALYTIC REACTORS

Description:

- Catalysed chemical reactions.
- Types of catalysis: homogeneous and heterogeneous.
- Catalysis and surface chemistry.
- Surface adsorption isotherms.
- Rate-determining steps in catalytic systems.
- Deactivation of catalysts.
- Microbial and enzymatic catalysis.

Specific objectives:

On completing this topic, students will be able to:

- Understand the catalytic systems used in modern industrial chemistry.
- Assess the parameters that must be considered in a catalytic system and the surface chemistry concepts that govern the system.
- Differentiate between the microbial and enzyme systems of chemical systems.
- Identify the transport mechanisms that govern reactor systems with catalysts, microorganisms and enzymes (suspended, encapsulated and/or immobilised).
- Determine which of the steps involved in a process is the rate-determining step.
- Understand the functioning of industrial catalysts with real examples.

Full-or-part-time: 20h

Theory classes: 8h

Laboratory classes: 2h

Self study : 10h

TOPIC 5: SOLID CATALYST REACTORS

Description:

- Effects of diffusion in heterogeneous reactions.
- Fundamentals of mass transfer.
- External resistance to mass transfer.
- Porous catalysts.
- Overall effectiveness factors.
- Multi-step reactors.
- Packed and fluidised beds.

Specific objectives:

On completing this topic, students will be able to:

- Understand the transport mechanisms that govern catalytic systems.
- Determine the influence of diffusion in porous and non-porous systems.
- Design packed-bed and fluidised-bed reactors.
- Apply mass transport concepts and equations in reaction systems.

Full-or-part-time: 20h

Theory classes: 5h

Laboratory classes: 5h

Self study : 10h

TOPIC 6: REAL REACTORS

Description:

- Residence time distribution (RTD) of chemical reactors.
- RTD in an ideal reactor for a single reaction.
- RTD in an ideal reactor for multiple reactions.

Specific objectives:

On completing this topic, students will be able to:

- Understand the differences between calculated reactors and real reactors.
- Define the parameters that allow change to be regulated.
- Relate the parameters of a real reactor with process parameters.
- Understand the various mathematical functions that define RTD.

Full-or-part-time: 15h

Theory classes: 7h

Guided activities: 4h

Self study : 4h

GRADING SYSTEM

- First examination: 35%
- Second examination: 35%
- Resolution and presentation of case studies: 20%
- Directed-activity project: 10%

All those students who suspend, want to improve note or can not attend the partial exam, will have the opportunity to examine the same day of the final exam. If the circumstances do not make it feasible that it is the same day as the final exam, the teacher responsible for the subject will propose, via the Atenea platform, that the aforementioned recovery test will be carried out another day, during class hours .

The new note of the recovery exam will replace the old one only in case it is higher.

For those students who meet the requirements and submit to the reevaluation examination, the grade of the reevaluation exam will replace the grades of all the on-site written evaluation acts (tests, midterm and final exams) and the grades obtained during the course for lab practices, works, projects and presentations will be kept.

If the final grade after reevaluation is lower than 5.0, it will replace the initial one only if it is higher. If the final grade after reevaluation is greater or equal to 5.0, the final grade of the subject will be pass 5.0.

EXAMINATION RULES.

Students will be expected to have passed Chemistry and Experimentation in Chemical Engineering.

BIBLIOGRAPHY

Basic:

- Fogler, H. Scott. Elementos de ingeniería de las reacciones químicas. 3ª ed. México: Pearson Educación, 2001. ISBN 9702600790.
- Levenspiel, Octave. Ingeniería de las reacciones químicas. 3ª ed. México: Limusa Wiley, 2004. ISBN 9681858603.
- Missen, Ronald W.; Mims, Charles A.; Saville, Bradley A. Introduction to chemical reaction engineering and kinetics. New York: Wiley, 1999. ISBN 0471163392.
- Santamaría, Jesús [et al.]. Ingeniería de reactores. Madrid: Síntesis, 1999. ISBN 847738665X.
- Schmidt, Lanny D. The engineering of chemical reactions. 2nd ed. New York: Oxford University Press, 2005. ISBN 0195169255.
- Butt, John B. Reaction kinetics and reactor design. 2nd ed. New York: Marcel Dekker, 2000. ISBN 0824777220.