Course guide
820522 - ERQQ - Chemical Reaction Engineering

Last modified: 14/06/2023

Unit in charge: Barcelona East School of 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

LECTURER

Coordinating lecturer: AURELIO CALVET TARRAGONA

Others: Primer quadrimestre:
AURELIO CALVET TARRAGONA - Grup: T1
FRANCISCO ESTRANY CODA - Grup: T1

Segon quadrimestre:
FRANCISCO ESTRANY CODA - Grup: M10
VICENÇ MARTI GREGORIO - Grup: M10

PRIOR SKILLS

Those ones established in accordance with the knowledge acquired about chemistry, physics, mathematics, thermodynamics, material transfer and heat transmission

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
CEQUI-19. Understand mass and energy balances, biotechnology, mass transfer, separation operations, chemical reaction engineering, the design of reactors, and the recovery and processing of raw materials and energy resources.
CEQUI-20. Analyse, design, simulate and optimise processes and products.

Transversal:
07 AAT N3. 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.

TEACHING METHODOLOGY

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LEARNING OBJECTIVES OF THE SUBJECT

Provide the fundamental knowledge of stoichiometry, kinetics and equilibrium of complex systems with chemical reactions multiple
Apply the knowledge acquired to design chemical reactors' installations with the most appropriate configuration for a specific reaction

STUDY LOAD

Type	Hours	Percentage
Hours large group	60,0	40.00
Self study	90,0	60.00

Total learning time: 150 h

CONTENTS

-Theme 1: Introduction to Chemical Reactors

Description:
The chemical reactor in the chemical industry. Criteria and techniques for the design of reactors. Definitions and general concepts. Relations of the stoichiometry. Stoichiometric models. Invariant of reaction.

Specific objectives:
To acquire knowledge for calculation of stoichiometric models of chemical reactions with multiple chemical equations, known initial and final composition of the reactant system.

Related activities:
Initial test
Exercises
Test of monitoring
Problems
Final Test
Study of the theory
First report of non-attendance work.

Full-or-part-time: 35h
Theory classes: 14h
Self study : 21h

-Theme 2: Homogeneous kinetics

Description:
Kinetics and chemical equilibrium. Definitions and general concepts. Calculation of equilibrium composition at reversible chemical reactions. Homogeneous kinetics non catalytical. Kinetic models based on the order of reaction. Differential methods for analyzing data. Integral Methods for analyzing data. Homogeneous kinetics catalytical. Mechanisms and kinetic equations of reactions catalyzed.

Specific objectives:
To acquire knowledge for calculation of kinetic equations of homogeneous chemical reactions from the experimental results by fitting kinetic models proposed.

Related activities:
Initial test
Exercises
Test of monitoring
Problems
Final Test
Study of the theory

Full-or-part-time: 40h
Theory classes: 16h
Self study : 24h

-Theme 3: Heterogeneous kinetics and applications

Description:
Heterogeneous kinetics non catalytical: definition and general concepts. The processes of matter transfer. Reactions fluid A / fluid B (liquid-gas) and transfer factors. Reactors of two fluid phases (liquid-gas). Reactions solid / fluid. Heterogeneous kinetics catalytic: solid catalysts and adsorption models. Physical model of porous catalyst. Kinetic equations in the hyperbolic models based on heterogeneous catalysis.

Specific objectives:
To acquire knowledge for calculation about heterogeneous kinetics equations of chemical reactions from the models used to address the study of reaction mechanisms.

Related activities:
Study of the theory

Full-or-part-time: 22h 30m
Theory classes: 9h
Self study : 13h 30m

-Theme 4: Ideal reactors

Description:
Batch reactor (BR). Calculating the volume in a BR from a reaction and a specific production needs. Macroscopic energy balance in a BR: Isothermal system / Non-isothermal system (adiabatic reaction). Continuous stirred tank reactor (CSTR). Comparison between a BR and a CSTR for the same reaction and the same productivity. Macroscopic energy balance in a CSTR: Isothermal system / Non-isothermal system. Static Stability Conditions in a CSTR. Tubular Reactor (TR). Comparison between a CSTR and a TR for the same reaction and the same productivity. Macroscopic energy balance in a TR (temperature profile): Isothermal system / Non-isothermal system. Applications.

Specific objectives:
To acquire knowledge for calculation and design of chemical reactors based on kinetic and stoichiometric models of the proposed chemical reaction, using the models of ideal chemical reactors.

Related activities:
Exercises
Problems
Study of the theory

Full-or-part-time: 30h
Theory classes: 12h
Self study : 18h

-Theme 5: Design of installations of industrial reactors

Description:
Association of reactors, optimization of the yield and selectivity. Conversion reaction in an installation of reactors in series. CSTR in series. TR in series. Series mixed. Recirculating in TR. Determination of the optimal recirculation for a tubular reactor. Comparison between systems of more than one combined reactor. Systems with Multiple Reactions (serial/parallel). Applications.

Specific objectives:
To acquire knowledge of optimization of design parameters of chemical reactor according to criteria of economic profitability, safety and the minimizing environmental impact.

Related activities:
Exercises
Problems
Study of the theory
Second report of non-attendance work

Full-or-part-time: 22h 30m
Theory classes: 9h
Self study : 13h 30m

GRADING SYSTEM

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EXAMINATION RULES.

The realization of the activities is subject to the academic regulations established by the Technical University of Catalonia

BIBLIOGRAPHY

Basic:
- Levenspiel, Octave. Ingeniería de las reacciones químicas [on line]. 3ª ed. México: Limusa Wiley, 2004 [Consultation: 23/11/2021]. Available on: http://ebookcentral.proquest.com/lib/upcatalunya-ebooks/detail.action?docID=5758266. ISBN 9681858603.
- González Velasco, Juan Ramón [et al.]. Cinética química aplicada. Madrid: Síntesis, 1999. ISBN 8477386668.
- Santamaría, Jesús [et al.]. Ingeniería de reactores. Madrid: Síntesis, 1999. ISBN 847738665X.

Complementary:
- Fogler, H. Scott. Elementos de ingeniería de las reacciones químicas. México, D.F. [etc.]: Pearson Educación, 2008. ISBN 9789702611981.
- Levenspiel, Octave. El Omnilibro de los reactores químicos. Barcelona: Reverté, 1986. ISBN 8429173366.