

UNIVERSIDAD DE CASTILLA - LA MANCHA GUÍA DOCENTE

1. General information

 Course: APPLIED CHEMICAL KINETICS
 Code: 57713

 Type: CORE COURSE
 ECTS credits: 6

 Degree: 344 - CHEMICAL ENGINEERING
 Academic year: 2023-24

 Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
 Group(s): 21

Year: 2

Main language: Spanish

Use of additional

languages:

Web site:

English Friendly: Y
Bilingual: N

Lecturer: YOLANDA DIAZ DE MERA MORALES - Group(s): 21							
Building/Office	Department	Phone	number	ber Email		Office hours	
Edificio Marie Curie, segunda planta, despach 2.05	O QUÍMICA FÍSICA	926052	2872	372 yolanda.diaz@uclm.es		Monday and Wednesday from 4 to 6pm. Tuesday and Thursday from 12 to 13h.	
Lecturer: MARIA REYES	LOPEZ ALAÑON - Group(s):	21					
Building/Office	Department	Phone number Email			Office hours		
Marie Curie (segunda planta))	QUÍMICA FÍSICA	926052	779	reyes.lopez@uclm.es		Tuesday and Wednesday: 10-12 h Thursday: 17-19 h	
Lecturer: ALBERTO NOTARIO MOLINA - Group(s): 21							
Building/Office	Department	Phone number	Email		Office hours		
Edificio Marie Curie, primera planta	QUÍMICA FÍSICA	6347	alberto.	notario@uclm.es	Monday from 10 a.m. to 1 p.m. Tuesday, Wednesday and Thursday from 10 a.m. to 11 a.m.		

2. Pre-Requisites

Those established in general for the Degree

3. Justification in the curriculum, relation to other subjects and to the profession

It is essential that the student acquire a solid knowledge of the bases of chemical kinetics and its application to Chemical Engineering. The subject intends that the student deepens the understanding of these concepts, completes them and acquires the necessary skills for their application to the practical cases that will be presented both in their professional future and when studying other subjects of the study plan. Specifically, this subject will address the description of the concepts of formal kinetics, the learning of the different mathematical methods that exist to solve the kinetic equations, the factors that influence the rate of the reaction, knowing the different types of chemical reactors used in industry, address the study of catalyzed reactions and the different types of catalysis in reactions of industrial interest, etc. Applied Chemical Kinetics is a compulsory subject that will be taught in the second semester of the second year

4. Degree competences achieved in this course

Course competences	
Code	Description
CB02	Apply their knowledge to their job or vocation in a professional manner and show that they have the competences to construct and justify arguments and solve problems within their subject area.
E24	Knowledge and / or ability to handle chemical analysis equipment and property characterization, and the basic instruments of a chemical laboratory.
E25	Manipulate chemicals safely and environmentally
E31	Basic knowledge of the principles of transport phenomena and the kinetic and thermodynamic aspects of chemical processes
G03	Knowledge in basic and technological subjects, which enables them to learn new methods and theories, and give them versatility to adapt to new situations.
G20	Ability to analyze and solve problems
G21	Ability to learn and work autonomously
G22	Ability to apply theoretical knowledge to practice

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Being able to simulate the concentration profiles of the species involved in a reacting chemical system.

To have the ability to autonomously work in a laboratory and skills in handling experimental techniques to obtain thermodynamic properties and the monitoring of kinetic processes.

To have knowledge and ability to manage bibliographic sources of thermodynamic and kinetic nature.

Have knowledge of the fundamentals of chemical kinetics and its application to Chemical Engineering.

Being able to integrate the thermodynamic and kinetic aspects of a chemical process.

6. Units / Contents

Unit 1: Introduction. Stoichiometric analysis of chemical reactions

Unit 1.1 Necessity and importance of stoichiometry in chemical processes: definition of stoichiometric model. Stoichiometric analysis in complex reactions: determination of key species, relationship between key and non-key species, determination of stoichiometric equations that represent the system.

Unit 2: Rate of chemical reactions. Elementary and complex reactions

Unit 2.1 Different ways to express reaction rate. Factors that affect the rate of reaction: pressure, temperature and composition. Elementary and complex reactions: mechanisms of complex reactions. Steady-state and rate-determining step approximation. Influence of temperature: Theory of collisions and transition state theory

Unit 3: Rate equations in constant volume batch reactors

Unit 3.1 Integrated rate laws in simple reactions of order 1, 2, order n. Half-life, Powell and isolation method to obtain the reaction order. Integrated rates in complex reactions: irreversible in series and in parallel. reversible reactions. differential method.

Unit 4: Rate equations in variable volume batch reactors

Unit 4.1 Definition of relative volume variation. Kinetic equation for variable volume batch reactors. Differential method of analysis. Integral method: zero order reactions, 1st order reactions and 2nd order reactions.

Unit 5: Kinetic equations in steady state flow reactors

Unit 5.1 Introduction. Time and spatial rate. Continuous stirred tank reactor. Plug flow reactor. Integrated rate equations for flow reactors.

Unit 6: Homogeneous catalysis

Unit 6.1 Differences between reactions in the liquid phase and in the gas phase. Introduce the phenomenon of catalysis. Homogeneous specific and general acid-base catalysis.

Unit 7: Heterogeneous catalysis

Unit 7.1 Non-catalytic heterogeneous reactions. Solid-fluid reactions. Introduce heterogeneous catalysis. Establish the different stages and activation energies and corresponding enthalpies. Study characteristics of heterogeneous catalysis and different adsorption isotherms. Introduce kinetics of enzymatic reactions (homogeneous and heterogeneous)

ADDITIONAL COMMENTS, REMARKS

Laboratory practices

Practice 1. Kinetics of hydration of acetic anhydride by a colorimetric method

Practice 2. Kinetics of hydrolysis of tert-butyl iodide by conductivity measurements

Practice 3. Glucose mutarotation kinetics by polarimetry

Practice 4.

7. Activities, Units/Modules and Methodology								
Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description	
Class Attendance (theory) [ON-SITE]	Lectures	CB02 E31 G03 G20 G21 G22	1.36	34	N	-		
Other off-site activity [OFF-SITE]	Self-study		1.96	49	Ν	-		
Workshops or seminars [ON-SITE]	Workshops and Seminars	CB02 E31 G03 G20 G21 G22	0.32	8	Υ	N		
Other off-site activity [OFF-SITE]	Self-study		0.52	13	Ν	-		
Laboratory practice or sessions [ON-SITE]	Practical or hands-on activities	CB02 E24 E25 E31 G03 G20 G21 G22	0.6	15	Υ	Υ		
Other off-site activity [OFF-SITE]	Self-study		0.88	22	N	-		
Final test [ON-SITE]	Assessment tests		0.12	3	Υ	Y		
Study and Exam Preparation [OFF-SITE]	Self-study		0.24	6	N	-		
Total:								
Total credits of in-class work: 2.4				Total class time hours: 60				
Total credits of out of class work: 3.6			Total hours of out of class work: 90					

As: Assessable training activity

Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System					
Evaluation System	Continuous assessment	Non- continuous evaluation*	Description		
Assessment of problem solving and/or case studies	25.00%	0.00%			
Final test	60.00%	85.00%			
Laboratory sessions	15.00%	15.00%			
Total:	100.00%	100.00%			

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject, an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

- 1. Exam with questions and problems about the contents taught (60%).
- 2. Continuous evaluation on learning based on practical cases, problems, questionnaires, etc... especially in the seminars (25%).
- 3. Continuous evaluation of the work in the laboratory, including the proper preparation of the results sheets (15%).

To make the average, a minimum of 4/10 in each of the 3 parts will be required. To pass the course, the overall average must be equal to or greater than 5/10.

Non-continuous evaluation:

Those students who report that they cannot follow the continuous assessment (and meet the established requirements), must do a final test where all the skills corresponding to the continuous assessment and the final exam (85% of the grade) will be evaluated.

The remaining 15% corresponds to laboratory practices.

To make the average it is required to obtain a minimum of 4/10 in each of these 2 parts. To pass the course, the overall average must be equal to or greater than 5/10.

Specifications for the resit/retake exam:

- 1. Examination of all the contents taught, including questions, cases and problems similar to those raised during the development of the course, including the seminars (85%).
- 2. Evaluation of the work in the laboratory including the preparation of the results sheets (15%). The lab note is kept for everyone. For those who have not passed a 4/10 in the ordinary call, this call will have an evaluation section of the corresponding competences that could be carried out in the laboratory. To make the average it is required to obtain a minimum of 4/10 in each of these 2 parts. To pass the course, the overall average must be equal to or greater than 5/10.
- There is no obligation to repeat the laboratory in the following course. In that case, the laboratory grade will be 4/10. If someone wants to repeat it, they can do it and the grade will be the one obtained in this case.

Specifications for the second resit / retake exam:

Similar to the first resit

9. Assignments, course calendar and important dates	
Not related to the syllabus/contents	
Hours	hours

10. Bibliography and Sources								
Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description		
I. N. Levine	Fisicoquímica	Mc Graw Hill			2004			
J. R González y colaboradores	Cinética Química Aplicada	Síntesis			1999			
O. Levenspiel	El omnilibro de los reactores químicos	Reverté			1986			
P. W. Atkins	Química Física	Omega			1999			
O. Levenspiel	Ingeniería de las reacciones químicas	Reverté			2000			