

**1. General information**

**Course:** EXPERIMENTAL TECHNIQUES OF KINETICS IN CHEMISTRY  
**Type:** CORE COURSE  
**Degree:** 2326 - MASTER DEGREE PROGRAMME IN CHEMICAL RESEARCH  
**Center:** 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY  
**Year:** 1

**Main language:** Spanish

**Use of additional languages:**

**Web site:**

**Code:** 310585

**ECTS credits:** 6

**Academic year:** 2019-20

**Group(s):** 20

**Duration:** C2

**Second language:** English

**English Friendly:** Y

**Bilingual:** N

| Lecturer: <b>ELENA JIMENEZ MARTINEZ</b> - Group(s): 20          |                |              |                           |  |
|---|----------------|--------------|---------------------------|--|
| Building/Office   | Department     | Phone number | Email                     | Office hours   |
| EDIFICIO MARIE CURIE, 2ª PLANTA                                 | QUÍMICA FÍSICA | 926052129    | elena.jimenez@uclm.es     | Monday, Tuesday and Wednesday: 13:30-14:30 16:00-17:00 |
| Lecturer: <b>ALBERTO NOTARIO MOLINA</b> - Group(s): 20          |                |              |                           |  |
| Building/Office   | Department     | Phone number | Email                     | Office hours   |
| Edificio Marie Curie, primera planta                            | QUÍMICA FÍSICA | 6347         | alberto.notario@uclm.es   | Monday, Tuesday and Wednesday: 11:30-13:30             |
| Lecturer: <b>FRANCISCO JAVIER POBLETE MARTIN</b> - Group(s): 20 |                |              |                           |  |
| Building/Office   | Department     | Phone number | Email                     | Office hours   |
| EDIFICIO MARIE CURIE 2ª PLANTA, DESPACHOS 2.03                  | QUÍMICA FÍSICA | 926052177    | fcojavier.poblete@uclm.es | Miércoles y Jueves: 9:00h-11:00h 12:30h-13:30h         |

**2. Pre-Requisites**

Not established

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

This subject is part of the Advanced Physical Chemistry Matter corresponding to Module I of this Master. The objective of the subject is to profound in the previously acquired knowledge of Chemical Kinetics in the Chemistry Degree, particularly in those that refer to the kinetics of fast reactions and experimental techniques that are currently used in the field of research for your study. Chemical Kinetics is one of the most active research areas in Physical Chemistry in both in homogeneous phase (solution or gas) and heterogeneous phase (gas-solid, gas-liquid and solid-liquid). The Kinetics of chemical reactions has great importance in industrial synthesis. Some of the applications of the kinetic study of fast reactions are the elucidation of the mechanisms and the rate of degradation of atmospheric pollutants, in the control of drugs and foods, in catalysis, etc.

**4. Degree competences achieved in this course****Course competences**

| Code | Description  |
|------|--|
| E07  | Knowing the principles of sustainable chemistry and safety standards for handling known chemicals  |
| E08  | Knowing the kinetics of chemical processes, including catalysis, reaction mechanisms and the methods and techniques used to determine them.  |
| G01  | Knowing the precision of the experimental data and its use for the planning of experimental research work.   |
| G02  | Having the necessary ability to perform advanced laboratory procedures and the use of instrumentation in synthetic and analytical work.  |
| T02  | Ability to work in a team and to exercise leadership functions, fostering the entrepreneurial character  |
| T04  | Ability to use specific software for research in chemistry.  |
| T05  | Ability to obtain bibliographic information at the research level, including Internet resources (databases, specialized scientific bibliography, social networks, etc ...), as well as carry out a selection and classification of it. |

**5. Objectives or Learning Outcomes****Course learning outcomes****Description**

- To apply knowledge about the methodologies used to obtain and analyze kinetic data.
- To apply the acquired knowledge to carry out a kinetic experiment in the laboratory.
- To apply detection methods in a heterogeneous experimental system.
- To obtain the kinetic rate coefficients
- To interpret the results of a kinetic or computational study and present them properly, supported by the information obtained from previous bibliographic search
- To use properly the main experimental techniques in the kinetic study of reactions
- To perform extra-kinetic tests in order to know the reaction mechanism

**Additional outcomes****6. Units / Contents**

Unit 1: TOPIC 1. KINETICS OF FAST REACTIONS. FLOW TECHNIQUES Continuous Flow Technique. Accelerated Flow Technique. Stopped Flow Technique. Application of the Stopped Flow Technique to reactions in the gas phase.

Unit 2: TOPIC 2. KINETICS OF FAST REACTIONS. RELAXATION TECHNIQUES Instantaneous perturbation: Instantaneous temperature and pressure jump. Shock tubes. Continuous and periodic perturbations.

Unit 3: TOPIC 3. KINETICS OF FAST REACTIONS. METHODS OF INITIATION THROUGH INTENSIVE RADIATIONS AND RESONANCE SPECTROSCOPIES. Flash Photolysis. Laser photolysis. Pulsed radiolysis. Nuclear Magnetic Resonance Spectroscopy. Electronic spin spectroscopy.

Unit 4: TOPIC 4. EXPERIMENTAL TECHNIQUES IN GAS-PHASE KINETICS. Initiation Systems of the Reaction. Reactors. Spectroscopic Detection Methods. Absolute and Relative Kinetic Techniques. Discharge Fast Flow Tube (DFF). Pulsed Photolysis / Laser Induced Fluorescence (PLP / LIF). Time Resolved Laser Diode Absorption Spectroscopy (TLDAS). Cavity Ring-down spectroscopy (CRDS). Structure-reactivity correlations. SAR method (structure-activity relationship)

Unit 5: TOPIC 5. EXPERIMENTAL TECHNIQUES IN WHICH AEROLS ARE INVOLVED. Importance of aerosols. Formation processes in the atmosphere. Experimental systems established to study heterogeneous reactions. New mass spectrometry techniques to study heterogeneous atmospheric processes. Techniques to characterize aerosols in the environment (optical properties of aerosols, atmospheric transport of aerosols, characterization by space means, terrestrial and suborbital platforms). Adsorption processes on different surfaces. Characterization of adsorption processes under equilibrium conditions. Mechanism of adsorption of gases on liquid surfaces. Experimental system to study heterogeneous reactions with ice and dust.

Unit 6: EXPERIMENT 1. KINETICS IN SOLUTION

Unit 7: EXPERIMENT 2. KINETICS OF THE REACTION OF THE RADICAL Cs BY PHOTOLYSIS PULSED AND INDUCED FLUORESCENCE PRO LASER. In this lab practice, the rate constant of a bimolecular reaction in gas phase (Cs + CFCl<sub>3</sub>) is determined. Cs is generated by UV photolysis of CsCl and the kinetic data are obtained by monitoring the laser-induced fluorescence of Cs at different reaction times.

Unit 8: EXPERIMENT 3. KINETICS OF NO<sub>3</sub> REACTION BY MEANS OF RELATIVE METHODS

Unit 9: EXPERIMENT 4. Characterization by means of the SMPS technique of the formation of secondary organic aerosols, SOA, from the reaction of ozonolysis of different organic compounds.

| 7. Activities, Units/Modules and Methodology |                                  |   |                                      |       |    |     |   |             |
|--|----------------------------------|---|--------------------------------------|-------|----|-----|---|-------------|
| Training Activity                            | Methodology                      | Related Competences<br>(only degrees before RD<br>822/2021) | ECTS                                 | Hours | As | Com | R | Description |
| Class Attendance (theory) [ON-SITE]          | Lectures                         | E08 G01 G02   | 1                                    | 25    | Y  | N   | Y |             |
| Workshops or seminars [ON-SITE]              | Problem solving and exercises    | E08 G01 G02 T04 T05   | 0.56                                 | 14    | Y  | N   | Y |             |
| Other off-site activity [OFF-SITE]           | Guided or supervised work        | E08 G01 T05   | 3.6                                  | 90    | Y  | Y   | Y |             |
| Laboratory practice or sessions [ON-SITE]    | Practical or hands-on activities | E07 T02 T04   | 0.52                                 | 13    | Y  | Y   | Y |             |
| Individual tutoring sessions [ON-SITE]       | Other Methodologies              |   | 0.2                                  | 5     | Y  | N   | Y |             |
| Progress test [ON-SITE]                      | Assessment tests                 | E08 G01 G02   | 0.04                                 | 1     | Y  | N   | Y |             |
| Final test [ON-SITE]                         | Assessment tests                 | E08 G01 G02   | 0.08                                 | 2     | Y  | Y   | Y |             |
| Total:                                       |                                  |   | 6                                    | 150   |    |     |   |             |
| 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

R: Rescheduling training activity

| 8. Evaluation criteria and Grading System             |                |                    |   |
|---|----------------|--------------------|---|
| Evaluation System                                     | Grading System |                    | Description   |
|   | Face-to-Face   | Self-Study Student |   |
| Progress Tests  | 20.00%         | 0.00%              | Evaluation of theoretical contents and exercises.       |
| Practicum and practical activities reports assessment | 20.00%         | 0.00%              | Continuous assessment of laboratory work and lab report |
| Assessment of problem solving and/or case studies     | 20.00%         | 0.00%              | Resolution of seminars and practical cases.             |
| Other methods of assessment                           | 10.00%         | 0.00%              | Tutorials   |
| Final test  | 30.00%         | 0.00%              | Test of the contents of each part of the subject.       |
| Total:  | 100.00%        | 0.00%              |   |

**Evaluation criteria for the final exam:**

The ones specified in the previous table.

Disclaimer:

The practical case proposed by the teaching team will be individually supervised throughout the semester. The student must submit a written report of that work and make an oral presentation of it.

**Specifications for the resit/retake exam:**

The qualifications of the laboratory work and the corresponding scientific report will be maintained in this extraordinary call.

| 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 |

| Equipo Docente            | APUNTES FACILITADOS POR<br>LOS PROFESORES      |                 |               | Disponibles en la<br>plataforma Moodle |
|---------------------------|--|-----------------|---------------|--|
| Finlayson-Pitts and Pitts | Chemistry of the upper and lower<br>atmosphere | Academic Press  |               | 2000                                   |
| LAIDLER, Keith J.         | Chemical kinetics                              | Harper & Row    | 0-06-043862-2 | 1987                                   |
| S. Senent.                | QUÍMICA FÍSICA II.                             | Uned.           |               | 1985                                   |
| S.R. Logan                | FUNDAMENTOS DE CINÉTICA<br>QUÍMICA             | Addison Wesley. |               | 1996                                   |