



Teaching Guide

| Identifying Data | | | | | 2022/23 |
|--------------------------|--|--------|--|---------|---------|
| Subject (*) | Chemical Speciation and Computation | Code | 610500015 | | |
| Study programme | Mestrado Universitario en Ciencias, Tecnoloxías e Xestión Ambiental (plan 2012) | | | | |
| Descriptors | | | | | |
| Cycle | Period | Year | Type | Credits | |
| Official Master's Degree | 2nd four-month period | First | Optional | 3 | |
| Language | SpanishGalician | | | | |
| Teaching method | Face-to-face | | | | |
| Prerequisites | | | | | |
| Department | Química | | | | |
| Coordinador | Sastre De Vicente, Manuel Esteban | E-mail | manuel.sastre@udc.es | | |
| Lecturers | Barriada Pereira, José Luis Sastre De Vicente, Manuel Esteban Vilariño Barreiro, Maria Teresa | E-mail | jose.barriada@udc.es manuel.sastre@udc.es teresa.vilarino@udc.es | | |
| Web | | | | | |
| General description | This course is oriented to provide an overview of the methods of calculation of the concentration and distribution of species in solution, the interactions appearing in solution and the relationship between speciation, bioavailability and toxicity. | | | | |

Study programme competences / results

| Code | Study programme competences / results |
|------|--|
| A1 | Coñecemento das realidades interdisciplinares da Química e do Medio Ambiente, dos temas punteiros nestas disciplinas e das perspectivas de futuro. |
| A3 | Capacitar ao alumno para o desenvolvemento dun traballo de investigación nun campo da Química ou do Medio Ambiente, incluíndo os procesos de caracterización de materiais, o estudo das súas propiedades fisicoquímicas e biolóxicas e dos procesos que poden sufrir no medio natural. |
| A6 | Coñecemento do comportamento de diferentes especies químicas e dos procesos aos que poden estar sometidas unha vez liberadas no medio ambiente, incluíndo as súas relacións entre distintos compartimentos ambientais. |
| A9 | Coñecer algunhas aplicacións básicas da química computacional e dos programas de cálculo máis utilizados nos ámbitos da química e o medio ambiente. |
| A10 | Relacionar a presenza de especies químicas no medio natural cos conceptos de toxicidade e biodisponibilidade. |
| A14 | Coñecer as principais propiedades fisicoquímicas das augas naturais, relacionalas coa súa calidade e entender as principais tecnoloxías de tratamento de augas naturais. |
| B1 | Posuír e comprender coñecementos que acheguen unha base ou oportunidade de ser orixinais no desenvolvemento e/ou aplicación de ideas, a miúdo nun contexto de investigación. |
| B2 | Que os estudantes saiban aplicar os coñecementos adquiridos e a súa capacidade de resolución de problemas en contornas novas ou pouco coñecidas dentro de contextos máis amplos (ou multidisciplinares) relacionados coa súa área de estudo. |
| B3 | Que os estudantes sexan capaces de integrar coñecementos e enfrontarse á complexidade de formular xuízos a partir dunha información que, sendo incompleta ou limitada, inclúa reflexións sobre as responsabilidades sociais e éticas vinculadas á aplicación dos seus coñecementos e xuízos. |
| B4 | Que os estudantes saiban comunicar as súas conclusións e os coñecementos e razóns últimas que as sustentan a públicos especializados e non especializados dun modo claro e sen ambigüedades. |
| B6 | Ser capaz de analizar datos e situacións, xestionar a información dispoñible e sintetizala, todo iso a un nivel especializado. |
| B8 | Comprender, a un nivel especializado, as consecuencias do comportamento humano na contorna ambiental. |
| C2 | Ser capaz de manter un pensamento crítico dentro dun compromiso ético e no marco da cultura da calidade. |
| C3 | Ser capaz de adaptarse a situacións novas, mostrando creatividade, iniciativa, espírito emprendedor e capacidade de liderado. |
| C4 | Expresarse correctamente, tanto de forma oral coma escrita, nas linguas oficiais da comunidade autónoma. |
| C5 | Dominar a expresión e a comprensión de forma oral e escrita dun idioma estranxeiro. |
| C6 | Utilizar as ferramentas básicas das tecnoloxías da información e as comunicacións (TIC) necesarias para o exercicio da súa profesión e para a aprendizaxe ao longo da súa vida. |



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| C9 | Valorar criticamente o coñecemento, a tecnoloxía e a información dispoñible para resolver os problemas cos que deben afrontarse. |
| C11 | Valorar a importancia que ten a investigación, a innovación e o desenvolvemento tecnolóxico no avance socioeconómico e cultural da sociedade. |

| Learning outcomes | | | |
|---|---------------------------------------|-------------------|---|
| Learning outcomes | Study programme competences / results | | |
| Ability to identify pollutants in natural water | AC3 | | |
| To calculate the concentrations and / or activities of molecular and ionic species in a natural water | AC6 | BC2 | |
| To provide useful thermodynamic data in studies of environmental impact of pollutant release on water sources | AC1 AC6 | BC2 BC6 | |
| To learn writing a full report (introduction, background, experimental part, description of results and discussion, conclusions and recommendations, bibliography) on studies of pollution by metals and other contaminants in the aquatic environment | | BC1 BC4 BC6 | CC4 |
| To extract relevant information derived from reading research articles about real problems associated with water pollution and / or modeling processes in natural waters; to summarize their content and judge them critically | AC1 AC6 AC14 | BC3 BC4 | CC2 CC3 CC5 CC6 CC9 CC11 |
| To knowing the structure of the speciation programs used in the calculation of chemical speciation problems. To be able to use at least one of these programs. To acquire the ability to apply mathematical equations and procedures necessary to solve the model leading to the calculation of water composition in terms of chemical speciation | AC9 | BC6 | |
| To learn judging critically the relationship between speciation, bioavailability and toxicity through the use of different models | AC9 AC10 | BC8 | |

| Contents | |
|---|---|
| Topic | Sub-topic |
| Chapter 1. Modeling of chemical equilibrium in natural waters | Main composition of natural water. Approach problem solving of chemical equilibrium: general methodology. Mass balances. Electro-neutrality condition. |
| Chapter 2. Ionic interactions in natural waters | Models of interaction: ionic association versus physical interaction. Models of activity coefficient of widely use in oceanography, geochemistry etc.. Surface complexation models. |
| Chapter 3. Examples: Acid-base, complexation, solubility and redox equilibria | Application of the general methodology for calculating speciation in the system CO ₂ /H ₂ O/calcite. Redox reactions and speciation. Other examples. |
| Chapter 4. Speciation and toxicity | The model of free ion activity. The biotic ligand model. The distribution coefficient octanol / water. Other models. |

| Planning | | | | |
|---------------------------------|-------------------------|--------------------------------------|-------------------------------|-------------|
| Methodologies / tests | Competencies / Results | Teaching hours (in-person & virtual) | Student?s personal work hours | Total hours |
| Guest lecture / keynote speech | A1 A6 A10 A14 | 7 | 21 | 28 |
| Supervised projects | A3 B1 B3 B4 B6 C4 C5 | 1 | 14 | 15 |
| Seminar | A9 C6 | 2 | 7 | 9 |
| Laboratory practice | B2 C3 C9 C11 | 11 | 0 | 11 |
| Events academic / information | B8 C2 | 0 | 2 | 2 |
| Mixed objective/subjective test | A6 A14 | 2.5 | 7.5 | 10 |
| Personalized attention | | 0 | | 0 |

(*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

| Methodologies | |
|---------------------------------|--|
| Methodologies | Description |
| Guest lecture / keynote speech | Classroom presentation of the subject |
| Supervised projects | Reading, analysis and discussion of research articles about modeling with emphasis in the field of environment |
| Seminar | Solving some of proposed. Any question/clarification that may arise in these sessions will be solved |
| Laboratory practice | Calculations of speciation of metals in water by using specific spreadsheet programs. The use of these programs will be explained to students |
| Events academic / information | Supplementary activities such as visits to a research laboratory, informative video projections, talks/communications in the faculty or thematic searches on the internet. |
| Mixed objective/subjective test | Examination of the subject contents |

| Personalized attention | |
|---|--|
| Methodologies | Description |
| Supervised projects Seminar Laboratory practice | <p>Students are recommended to use individualized tutoring to solve all questions, issues and concepts that are not clear concerning the contents of the subject.</p> <p>Practices (in laboratory and computer room) will be made ??with the constant presence of the teachers who will resolve individually all questions and concerns that may arise from each student.</p> <p>Official dates of personalized attention: Tuesdays and Thursdays from 10 to 13 h.</p> <p>In any case, during the week students can rise any questions related to the subject.</p> |

| Assessment | | | |
|---------------------------------|------------------------|---|---------------|
| Methodologies | Competencies / Results | Description | Qualification |
| Supervised projects | A3 B1 B3 B4 B6 C4 C5 | Delivery and presentation a short summary of the article/s assigned on modeling and calculations of speciation. | 5 |
| Seminar | A9 C6 | Delivery of one of the problems proposed in class. | 5 |
| Laboratory practice | B2 C3 C9 C11 | Compulsory attendance to all practices in the computer room and delivery of a summary of the work performed. | 20 |
| Mixed objective/subjective test | A6 A14 | Exam of the contents. | 70 |

| Assessment comments |
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| Sources of information | |
|------------------------|--|
| Basic | A.M.URE,C.M.DAVIDSON eds. Chemical Speciation in theEnvironment. 2ª ed. Blackwell 2002 A TESSIER,D.R.TURNER eds. Metal Speciation andbioavailability in Aquatic Systems. IUPAC Series on Analytical, PhysicalChemistry and Environmental Systems. Vol. 23. Wiley 1995.FRANCOIS M.M. MOREL; JANET G. HERING (1993).Principles and Applications of Aquatic Chemistry. John Willey & Sons,New York STUMM,W. & MORGAN, J.J (1996). Aquatic Chemistry. John Willey & Sons. |
| Complementary | |



| Recommendations |
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| Subjects that it is recommended to have taken before |
| Subjects that are recommended to be taken simultaneously |
| Subjects that continue the syllabus |
| Other comments |
| Prerequisite knowledge: Graduates in Science and/or Engineering. |

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.