Teaching Guide				
Identifying Data				2017/18
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	Optativa	3
Language	SpanishGalician			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Sastre De Vicente, Manuel Esteban	E-mail	manuel.sastre@udc.es	
Lecturers	Sastre De Vicente, Manuel Esteban	E-mail	manuel.sastre@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	
Code	Study programme competences
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 coñecidos 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 suizos.
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.
C9	Valorar criticamente o coñecemento, a tecnoloxía e a información dispoñible para resolver os problemas cos que deben enfrontarse.

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		
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 CO2/H2O/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	Ordinary class hours	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	Students are recommended to use individualized tutoring to solve all questions, issues and concepts that are not clear concerning the contents of the subject. 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. Official dates of personalized attention: Tuesdays and Thursdays from 10 to 13 h. In any case, during the week students can rise any questions related to the subject.

Assessment			
Methodologies	**Competencies**	**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

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
Subjects that it is recommended to have taken before

Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments
Prerequisit 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.