Course guides
2500207 - GECTERCIAM - Environmental Thermodynamics and Kinetics

Unit in charge: Barcelona School of Civil Engineering
Teaching unit: 751 - DECA - Department of Civil and Environmental Engineering.
Degree: (ANG) GRAU EN ENGINYERIA AMBIENTAL (Syllabus 2020). (Compulsory subject).
Academic year: 2020 ECTS Credits: 6.0 Languages: Catalan, Spanish, English

LECTURER
Coordinating lecturer: PAULA - FELICIDAD RODRIGUEZ ESCALES
Others: PAULA - FELICIDAD RODRIGUEZ ESCALES

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
14446. Solve mathematical problems that may arise in engineering by applying knowledge about: linear algebra, geometry, differential geometry, differential and integral calculus, optimization, ordinary differential equations.
14447. Obtain basic knowledge about the use and programming of computers, operating systems, databases and basic numerical calculation and applied to engineering.
14448. Manage the basic concepts about the general laws of mechanics and thermodynamics, concept of field and heat transfer, and apply them to solve engineering problems.
14449. Apply the basic principles of general chemistry, organic and inorganic chemistry and their applications in engineering.
14450. Describe the global functioning of the planet: atmosphere, hydrosphere, lithosphere, biosphere, anthroposphere, biogeochemical cycles (C, N, P, S), soil morphology and apply it to problems related to geology, geotechnics, edaphology and climatology.

General:
14440. Identify, formulate and solve problems related to environmental engineering.
14441. Apply the functions of consulting, analysis, design, calculation, project, construction, maintenance, conservation and exploitation of any action in the territory in the field of environmental engineering.
14444. Apply business management techniques and labor legislation.

TEACHING METHODOLOGY

The course consists of 2 hours per week of classroom activity (large size group) and 1 hour weekly with half the students (medium size group).

The 2 hours in the large size groups are devoted to theoretical lectures, in which the teacher presents the basic concepts and topics of the subject, shows examples and solves exercises.

The 1 hour in the medium size groups is devoted to solving practical problems with greater interaction with the students. The objective of these practical exercises is to consolidate the general and specific learning objectives.

The rest of weekly hours devoted to laboratory practice.

Support material in the form of a detailed teaching plan is provided using the virtual campus ATENEA: content, program of learning and assessment activities conducted and literature.
LEARNING OBJECTIVES OF THE SUBJECT


1. Understand the laws of thermodynamics that govern the phenomena of transformation and transfer of energy and study of thermodynamics of colloidal surfaces and systems.
2. Study chemical kinetics and equilibrium in multicomponent systems.
3. Understand the concepts of transience, adsorption, reaction mechanisms, solution reaction, environmental catalysis, oxidation-reduction processes and enzymatic activity. Application to the design of reactors.

Environmental Thermodynamics and Kinetics. Study of the laws of thermodynamics and chemical kinetics to understand fundamental concepts for the design of reactors such as adsorption, transience, enzymatic activity, oxidation-reduction processes, etc.

STUDY LOAD

<table>
<thead>
<tr>
<th>Type</th>
<th>Hours</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Hours small group</td>
<td>15,0</td>
<td>10.00</td>
</tr>
<tr>
<td>Hours medium group</td>
<td>15,0</td>
<td>10.00</td>
</tr>
<tr>
<td>Self study</td>
<td>84,0</td>
<td>56.00</td>
</tr>
<tr>
<td>Guided activities</td>
<td>6,0</td>
<td>4.00</td>
</tr>
<tr>
<td>Hours large group</td>
<td>30,0</td>
<td>20.00</td>
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</tbody>
</table>

Total learning time: 150 h

CONTENTS

T1. Basic concepts of classical thermodynamics

Description:
In this class the basic concepts of thermodynamics will be introduced. The concept of heat and work will be worked on. This session will explain the first principle of thermodynamics, the concept of internal energy and enthalpy. The second principle of thermodynamics with the concept of entropy will also be explained. Application of the first and second principles to the behavior of ideal gases.
Third principle and postulates.
During this session there will be problems with each topic, the prob

Specific objectives:
Introduction to the basic concepts of thermodynamics. Introduce the concepts of heat and work. Introduce basic concepts of thermometry.
Know the state functions of classical thermodynamics.
Definition of the Gibbs equation. Maxwell’s relations.
Practice and deepen the knowledge of each topic.

Full-or-part-time: 24h
Theory classes: 6h
Practical classes: 4h
Self study: 14h
### T2. Single-component phase diagrams and pure substances

**Description:**
Phase rule. Phase diagrams and Clapeyron equation. Thermochemistry. Calorimetry. Standard conditions. Database. During this session there will be problems with each topic. The teacher will perform an example problem and the rest for the students with the support of the teacher.

**Specific objectives:**
Understand single-component phase diagrams. Calculate the vapor pressure in equilibrium at different temperatures. Know the thermodynamic properties of the formation of a single component: enthalpies, entropies, heat capacity and operate with them. Hess's law. Deepen the knowledge explained in the topic.

**Full-or-part-time:** 14h 23m  
Theory classes: 4h  
Practical classes: 2h  
Self study: 8h 23m

### T3. Mixtures and solutions

**Description:**
Mixtures and solutions. Partial molar magnitudes. Mixing magnitudes. Determination of partial molar magnitudes. Dissolution heats. 3.6 Ideal solutions and ideally diluted solutions 3.7 Colligative properties  
During this session there will be problems with each topic. The teacher will perform an example problem and the rest for the students with the support of the teacher.

**Specific objectives:**
Know the partial molar magnitudes. Calculate enthalpy / entropy / free energy of the mixture. Introduction to the concept of chemical potential.  
Deepen the knowledge of the subject.

**Full-or-part-time:** 19h 12m  
Theory classes: 4h  
Practical classes: 4h  
Self study: 11h 12m


**Description:**  
Closed systems of variable composition. Chemical potential. Non-ideal solutions. Determination of activity and activity coefficients. Definition of activity and activity coefficients in ionic solutions. Definition of ionic strength. Debye-Hückel theory. During this session there will be problems with each topic. The teacher will perform an example problem and the rest for the students with the support of the teacher.

**Specific objectives:**
Calculate the activity coefficients in real solutions. Determine solute activity coefficients of ionic solutions. Know how to know the ionic strength.  
To deepen in the knowledge of the concepts explained in this subject.

**Full-or-part-time:** 19h 12m  
Theory classes: 4h  
Practical classes: 4h  
Self study: 11h 12m
T5. Chemical equilibrium of real solutions.

Description:
Material balance. Chemical equilibrium in ideal gases. Chemical equilibrium in real solutions. Chemical equilibrium of non-electrolyte solutions. Chemical balance of electrolytes. Chemical equilibrium of pure solids or liquids. Formation of complexes. During this session there will be problems with each topic. The teacher will perform an example problem and the rest for the students with the support of the teacher.

In this session students will be approached with geochemical codes that allow the calculation of the thermodynamic properties of real solutions.

Specific objectives:
Know how to apply chemical balance to different situations.
Know how to perform equilibrium calculations with real ionic solutions. Define mineral saturation, precipitation and dissolution indices. Formation of complexes. Deepen the knowledge of the concepts explained in each topic.
Know advanced tools for calculating specs.

Full-or-part-time: 28h 47m
Theory classes: 4h
Practical classes: 4h
Laboratory classes: 4h
Self study: 16h 47m


Description:
Redox systems. Electromotive force. Electrochemical potential. Nernst's law. During this session there will be problems with each topic. The teacher will perform an example problem and the rest for the students with the support of the teacher.

Specific objectives:
Familiarize yourself with reduction-oxidation systems. Calculations with Nernst's Law. Deepen in learning the concepts explained in the topic.

Full-or-part-time: 14h 23m
Theory classes: 4h
Practical classes: 2h
Self study: 8h 23m

T7. Chemical kinetics.

Description:
Kinetics versus balance. Chemical reactions and reaction rates. Temperature dependence of reaction rates. Reactions catalyzed by microorganisms. Microbial kinetics. During this session there will be problems with each topic. The teacher will perform an example problem and the rest for the students with the support of the teacher.

Specific objectives:
Apply kinetics depending on the type of reaction. Know the relationship between the kinetic constant and temperature. Deepen the knowledge explained in the topic.

Full-or-part-time: 14h 23m
Theory classes: 4h
Practical classes: 2h
Self study: 8h 23m
Inverted class

**Full-or-part-time:** 9h 36m  
Laboratory classes: 4h  
Self study : 5h 36m

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**GRADING SYSTEM**

The mark of the course is obtained from the ratings of continuous assessment and their corresponding laboratories and/or classroom computers.

Continuous assessment consist in several activities, both individually and in group, of additive and training characteristics, carried out during the year (both in and out of the classroom).

The teachings of the laboratory grade is the average in such activities.

The evaluation tests consist of a part with questions about concepts associated with the learning objectives of the course with regard to knowledge or understanding, and a part with a set of application exercises.

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**EXAMINATION RULES.**

Not performing a continuous assessment activity implies having a 0 in that activity. The first partial exam will eliminate subject as long as the grade is higher than 3.

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**BIBLIOGRAPHY**

**Basic:**

**Complementary:**