Course guides
250332 - TERMOPRONA - Thermodynamics of Natural Processes

Unit in charge: Barcelona School of Civil Engineering
Teaching unit: 1004 - UB - (ENG)Universitat de Barcelona.
Degree: BACHELOR'S DEGREE IN GEOLOGICAL ENGINEERING (Syllabus 2010). (Compulsory subject).

Academic year: 2020  ECTS Credits: 4.5  Languages: Catalan, English

LECTURER

Coordinating lecturer: NEUS OTERO PÉREZ
Others: NEUS OTERO PÉREZ

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
4026. Ability to apply methodologies for studying and assessing environmental impact, and, in general, environmental technologies, sustainability and waste disposal
4066. Ecology and regional development. Town and country planning and management

Generic:
3103. Students will learn to identify, formulate and solve a range of engineering problems. They will be expected to show initiative in interpreting and solving specific civil engineering problems and to demonstrate creativity and decision-making skills. Finally, students will develop creative and systematic strategies for analysing and solving problems.
3106. Students will learn to assess the complexity of the problems examined in the different subject areas, identify the key elements of the problem statement, and select the appropriate strategy for solving it. Once they have chosen a strategy, they will apply it and, if the desired solution is not reached, determine whether modifications are required. Students will use a range of methods and tools to determine whether their solution is correct or, at the very least, appropriate to the problem in question. More generally, students will be encouraged to consider the importance of creativity in science and technology.
3107. Students will learn to identify, model and analyse problems from open situations, consider alternative strategies for solving them, select the most appropriate solution on the basis of reasoned criteria, and consider a range of methods for validating their results. More generally, students will learn to work confidently with complex systems and to identify the interactions between their components.
3109. Students will learn to plan, design, manage and maintain systems suitable for use in civil engineering. They will develop a systematic approach to the complete life-cycle of a civil engineering infrastructure, system or service, which includes drafting and finalising project plans, identifying the basic materials and technologies required, making decisions, managing the different project activities, performing measurements, calculations and assessments, ensuring compliance with specifications, regulations and compulsory standards, evaluating the social and environmental impact of the processes and techniques used, and conducting economic analyses of human and material resources.
3112. Students will develop an understanding of the different functions of engineering, the processes involved in the life-cycle of a construction project, process or service, and the importance of systematising the design process. They will learn to identify and interpret the stages in preparing a product design specification (PDS), draft and optimise specifications and planning documents, and apply a systematic design process to the implementation and operation phases. Students will learn to write progress reports for a design process, use a range of project management tools and prepare final reports, and will be expected to show an awareness of the basic economic concepts associated with the product, process or service in question.
3113. Students will learn to identify user requirements, to draft definitions and specifications of the product, process or service in question, including a product design specification (PDS) document, and to follow industry-standard design management models. Students will be expected to show advanced knowledge of the steps involved in the design, execution and operation phases and to use the knowledge and tools covered in each subject area to the design and execution of their own projects. Finally, students will assess the impact of national, European and international legislation applicable to engineering projects.
Transversal:
585. ENTREPRENEURSHIP AND INNOVATION - Level 1. Showing enterprise, acquiring basic knowledge about organizations and becoming familiar with the tools and techniques for generating ideas and managing organizations that make it possible to solve known problems and create opportunities.
586. ENTREPRENEURSHIP AND INNOVATION - Level 2. Taking initiatives that give rise to opportunities and to new products and solutions, doing so with a vision of process implementation and market understanding, and involving others in projects that have to be carried out.
589. SUSTAINABILITY AND SOCIAL COMMITMENT - Level 2. Applying sustainability criteria and professional codes of conduct in the design and assessment of technological solutions.
594. TEAMWORK - Level 3. Managing and making work groups effective. Resolving possible conflicts, valuing working with others, assessing the effectiveness of a team and presenting the final results.
584. THIRD LANGUAGE. Learning a third language, preferably English, to a degree of oral and written fluency that fits in with the future needs of the graduates of each course.

TEACHING METHODOLOGY
The classes will be encouraged to maximize student participation. A detailed schedule of the subject and recommended reading material for each topic will be available in the virtual campus of UB. Regular attendance to class is very important to pass the course. Classes will be distributed as follows:
- Lectures of one hour. It is recommended to review the material and read the literature before each session begins.
- Problems, two-hour sessions focused on solving exercises related to theoretical content.
- Specific problem sessions of one or two hours in the computer room focused on the use of software and thermodynamic databases to solve problems.

During the course additional activities will be proposed at the virtual campus of the University of Barcelona, to enhance learning, the student must consult this space to follow the course and participate in the proposed activities.

LEARNING OBJECTIVES OF THE SUBJECT
Students will acquire a basic understanding of chemical thermodynamics and learn how it applies to environmental engineering problems.

Upon completion of the course, students will be able to: 1. Use simple equilibrium thermodynamics methods and techniques to analyse the stability of natural systems, focusing on the interactions of rocks and minerals with water and air in different environmental conditions and the interaction of public works materials with water and air.

Principles and postulates of equilibrium thermodynamics; Functions and equations of state; Thermal, mechanical and chemical equilibrium; Phase rule; Ideal gas as a reference model; Gibbs free energy; Standard thermodynamic properties of minerals and organic species in solution; Partial molar properties; Chemical potential; Aqueous solutions; Speciation; Ionic strength and activities; The equilibrium constant; Ionic product and saturation index; Influence of pH on natural systems; Natural oxidation-reduction processes; Applications in engineering: Acidic water, salt water, durability of public works, waste deposition; Mineral stability diagrams: Activities, Eh(pe)-pH, partial pressure; Stability at high temperatures and pressures; Binary and ternary phase diagrams; Thermodynamic databases in mineralogy and geochemistry

STUDY LOAD

<table>
<thead>
<tr>
<th>Type</th>
<th>Hours</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Practical classes</td>
<td>15,0</td>
<td>13.33</td>
</tr>
<tr>
<td>Theory classes</td>
<td>19,5</td>
<td>17.33</td>
</tr>
<tr>
<td>Laboratory classes</td>
<td>10,5</td>
<td>9.33</td>
</tr>
<tr>
<td>Self study</td>
<td>63,0</td>
<td>56.00</td>
</tr>
<tr>
<td>Guided activities</td>
<td>4,5</td>
<td>4.00</td>
</tr>
</tbody>
</table>

Total learning time: 112.5 h
## CONTENTS

### Item 1 Fundamentals

**Description:**
Definitions of systems (open, closed, isolated). Definition of states of equilibrium (metastable stable). Definitions of types of processes or reactions (reversible or irreversible). Intensive and extensive parameters. Partial molar properties. Phases and Components.

**Specific objectives:**
Get used to the basic terms.

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

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### Problems

**Description:**
Problems
- Properties of water. Simple Phase diagrams.
- Problems: Ideal Solutions, fugacity and activity.
- Problem: The equilibrium constant.
- Problem: Real solutions. Rule of the phases.
- Problem: Redox reactions.
- Problems: Solid Solutions.
- Rock-water systems.
- Phase diagrams.
- Practices: Thermodynamic Databases.

**Full-or-part-time:** 48h
- Practical classes: 20h
- Self study: 28h

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### Item 2 Thermodynamics of solutions

**Description:**
Reactions at equilibrium. The equilibrium constant (K). K in solid-solid reactions. Changes of K with temperature.
Partial molar volumes. Apparent molar volumes. Enthalpy, heat capacity and Gibbs energy.

**Full-or-part-time:** 12h
- Theory classes: 5h
- Self study: 7h

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### Evaluation

**Full-or-part-time:** 12h
- Laboratory classes: 5h
- Self study: 7h
**Topic 3 Applications**

**Description:**
Activities of the ionic species.
Mineral stability diagrams. Metastable phases.

**Full-or-part-time:** 16h 48m
Theory classes: 7h
Self study : 9h 48m

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**Item 4 Phase diagrams**

**Description:**

**Full-or-part-time:** 4h 48m
Theory classes: 2h
Self study : 2h 48m

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**Topic 5: Thermodynamic databases.**

**Description:**
NIST Chemistry WebBook, NASA Glenn database Thermodynamics

**Full-or-part-time:** 4h 48m
Theory classes: 2h
Self study : 2h 48m
GRADING SYSTEM

Continuous assessment.

- Partial tests (3 tests). The final grade is the average of 3 tests. In the case of not attending to one of the test scheduled for the continuous assessment, the final grade of the course will be "No show". (70% grade)

- Problems and practices. Assignments will be proposed in the virtual campus. The assignments should be submitted on time and are compulsory for the continuous assessment. An assignment not submitted on time (or not submitted at all) will be considered as zero mark (20% grade).

- Supervised assignment (10% grade).

Single examination.

The student who wants choose this option must request it in writing within 3 weeks from the start of course.

- Single-exam (90% grade).
- Supervised assignment (10% grade).

Criteria for re-evaluation qualification and eligibility: Students that failed the ordinary evaluation and have regularly attended all evaluation tests will have the opportunity of carrying out a re-evaluation test during the period specified in the academic calendar. Students who have already passed the test or were qualified as non-attending will not be admitted to the re-evaluation test. The maximum mark for the re-evaluation exam will be five over ten (5.0). The non-attendance of a student to the re-evaluation test, in the date specified will not grant access to further re-evaluation tests. Students unable to attend any of the continuous assessment tests due to certifiable force majeure will be ensured extraordinary evaluation periods.

These tests must be authorized by the corresponding Head of Studies, at the request of the professor responsible for the course, and will be carried out within the corresponding academic period.

BIBLIOGRAPHY

Basic:

Complementary: