Course guide
2500009 - GECQUIMMAT - Chemistry of Materials

Unit in charge: Barcelona School of Civil Engineering
Teaching unit: 751 - DECA - Department of Civil and Environmental Engineering.
Degree: BACHELOR’S DEGREE IN CIVIL ENGINEERING (Syllabus 2020). (Compulsory subject).
Academic year: 2022 ECTS Credits: 6.0 Languages: Catalan, English

LECTURER
Coordinating lecturer: SUSANA VALLS DEL BARRIO
Others: ANDREU CODINA MENDOZA, IGNACIO SEGURA PÉREZ, ISAAC TAN BACHS, SUSANA VALLS DEL BARRIO

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES
Specific:
14399. Theoretical and practical knowledge of the chemical, physical, mechanical and technological properties of the materials most used in construction. (Common module to the Civil branch)

TEACHING METHODOLOGY
The course consists of 2 hours per week of classroom activity (large size group) and 1.6 hours 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 1.6 hours 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.

To do the laboratory practices you need the following personal protective equipment (PPE):
* Blue lab coat UPC Mechanical
* Protection gloves - Mechanical
* Safety glasses
* Mechanical Kit (bluelab coat + protection gloves + safety glasses)
LEARNING OBJECTIVES OF THE SUBJECT

Knowledge of the chemical and physical properties of building materials. Basic knowledge of the structure of the material that allow the interpretation of the chemical, physical and mechanical properties of the materials from atomic interactions, as well as the establishment of relationships between their microscopic structure and their macroscopic properties. Structure, type and basic properties of the most common construction materials, as well as the degradation processes that these may suffer. Experimental techniques for determining the composition and structure of building materials.

1 Ability to identify, obtain the composition and structure of construction materials, through different experimental techniques.
2 Ability to design a material analysis program for a structure or infrastructure.
3 Ability to perform a critical assessment of the results of the material analysis program conducted in a structure.

Theoretical and practical knowledge of the chemical, physical, mechanical and technological properties of the materials most used in construction. Basic scientific knowledge of the chemistry of materials (heat, equilibrium, atomic order, crystals, polymers, and gels). Knowledge of structure, types and properties of construction materials (binders, phase diagrams, corrosion). Knowledge of the experimental methods of determining the composition and structure of construction materials.

Basic scientific knowledge of material chemistry (atomic structure, atomic classification, phase diagrams, reaction balance, reaction heat, reaction (chemical attack (corrosion, sulfatic attack, chlorides...). Knowledge of the structure and its balance, composition or basic components (conglomerates, alloys (steels)), type and study of the basic properties (chemical, physical and mechanical) of building materials.

Knowledge of experimental methods for determining the composition and structure (DRX) of building materials. Capacity and application of the Control and Safety Regulation (UNE, ASTM...) and the quality of building materials, and understanding of their fundamentals. To establish and consolidate the fundamental concepts of basic chemistry acquired in secondary (high school).

In the event that such knowledge has not been obtained, provide tools for students to achieve it and to correctly follow the subject. Provide basic knowledge of the structure of matter to interpret the chemical, physical and mechanical properties of materials from atomic interactions, to establish the relationship between microscopic structure and macroscopic properties.

Study the main types of chemical processes, influence factors and consequences that follow. Provide basic knowledge to understand the chemistry of the most common building materials, as well as the processes they may undergo. In conclusion, the basics of physical-chemical processes in which behavior and durability are regulated under different conditions of service of the most commonly used building materials in civil engineering.

STUDY LOAD

<table>
<thead>
<tr>
<th>Type</th>
<th>Hours</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hours large group</td>
<td>30,0</td>
<td>20.00</td>
</tr>
<tr>
<td>Guided activities</td>
<td>6,0</td>
<td>4.00</td>
</tr>
<tr>
<td>Self study</td>
<td>84,0</td>
<td>56.00</td>
</tr>
<tr>
<td>Hours medium group</td>
<td>24,0</td>
<td>16.00</td>
</tr>
<tr>
<td>Hours small group</td>
<td>6,0</td>
<td>4.00</td>
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Total learning time: 150 h

CONTENTS

Fundamental concepts of chemistry and Atomic Structure

Description:

Establish and consolidate the fundamental concepts of chemistry acquired in high school. In the event that this knowledge is not available, provide tools so that they can achieve it and allow the correct follow-up of the subject. The following basic knowledge is considered for the correct follow-up of the subject: - Formulation: to know the symbols and the valences of the main chemical elements; know how to formulate the most common inorganic compounds; recognize the different types of inorganic compounds (oxides, peroxides, hydroxides, hydrides, hydricid acids, oxacic acids and salts). - Stoichiometry: know and differentiate the
concepts of element, molecule, compound, ion; understand the concepts of atomic mass, molecular mass, mol, empirical formula and molecular formula; be able to perform simple stoichiometric calculations, limiting reagent calculation and performance of a reaction. - Gases and solutions: characteristics of the gaseous state; real gases and ideal gases; law of ideal gases; calculations and units of concentrations of solutions.

Atomic structure
Fundamental laws of chemistry
Bohr Models
Quantum mechanical model: quantum numbers, electronic configuration
The Periodic Table
Atomic periodic properties

Bond energy
Bond distance
Primary bonds: ionic bond, covalent bond, metallic bond
Intermolecular forces: Van der Waals bond, Hydrogen bond

Properties
Definition and classification of solids
Crystalline solids
Crystalline structure
Imperfections in solids
Amorphous solids
Graphical representations of equilibrium: phase diagrams
Binary systems: Isomorphous systems and eutectic systems.
Lever rule Quantification of phases and compositions.
Microstructure phases
Quantification phase diagrams: Alloys
Binary systems: isomorphous systems and eutectic systems
Lever rule: Quantification of phases and compositions.
Microstructure: Alloys
Preparation, analysis and identification of samples by the X-ray diffraction technique

Specific objectives:
Establish and consolidate the fundamental concepts of chemistry acquired in high school. In the event that this knowledge is not available, provide tools so that they can achieve it and allow the correct follow-up of the subject. The following basic knowledge is considered for the correct follow-up of the subject: - Formulation: to know the symbols and the valences of the main chemical elements; know how to formulate the most common inorganic compounds; recognize the different types of inorganic compounds (oxides, peroxides, hydroxides, hydrides, hydracidic acids, oxacic acids and salts). - Stoichiometry: know and differentiate the concepts of element, molecule, compound, ion; understand the concepts of atomic mass, molecular mass, mol, empirical formula and molecular formula; be able to perform simple stoichiometric calculations, limiting reagent calculation and performance of a reaction. - Gases and solutions: characteristics of the gaseous state; real gases and ideal gases; law of ideal gases; calculations and units of concentrations of solutions.

Provide basic knowledge of the structure of matter that allows the interpretation of the chemical, physical and mechanical properties of materials from atomic interactions, as well as the establishment of relationships between their microscopic structure and their macroscopic properties.

From the bonds define types of solids and their chemical properties
From the study of the crystal structure we delve into the imperfections that allow us to define solid solutions and from here we can define and understand alloys such as steel.

Knowledge of phase diagrams is vital to understanding and predicting the mechanical properties of an alloy. Phase diagrams allow us to relate composition and temperature to define a particular microstructure of the alloy in question.

Problem solving of different binary systems with components of metallic elements in order to determine different types of alloys describing microstructures, physical, chemical and mechanical properties of each alloy in question.

Knowledge of an instrumental analysis technique in the characterization of samples: X-ray diffraction. In order to complement and assimilate the contents explained in the classroom and thus enhance the activity of the student outside the classroom for a learning of skills. Student learning is more powerful and meaningful, and the skills learning skills, richer and more diverse, more creative and divergent, that is, much higher compared to the convergent-memoristic style.

Full-or-part-time: 38h 24m
Theory classes: 7h
Practical classes: 7h
Laboratory classes: 2h
Metallic materials and their durability

Description:
Classification and properties of metallic elements and metallic materials
Types of alloys: steel alloys and non-steel alloys
Defining phases of the Fe-Fe3C diagram
Steel alloys: Hypoeutectoid, Eutectoid, Hypereutectoid
Microstructure of steel alloys
Influence of the other elements in the Fe-C system
Quantification of phases and composition of alloys
Redox reaction. oxidation - reduction
Electrochemical battery/cells
Half-reaction potentials: reduction potentials
Nernst Equation

Oxidation states
Oxidation-reduction reactions
Nernst equation
Electrochemical heterogeneities
Mechanisms of corrosion by contact with oxygen: dry and wet corrosion.
Corrosion of materials for reinforced concrete: mechanism, protection methods.
Chemical protection: passivation
Carbonation and chloride corrosion mechanism
Service life: Tuutti diagram

Specific objectives:
Introduce to the study of one major construction materials used by the Civil Engineer in his professional exercise, from the study of the metallic materials or steel.
Basic knowledge of steels, classification, properties, raw materials.
Knowledge of one of the most important or main pathologies that civil engineering suffers today.
Corrosion is one of the main pathologies of reinforced concrete. Knowledge of the attack process and ways of protection to increase the useful life of the material and the structure.

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

Binders

Description:
The first binders: clay, gypsum and lime.
1- Clay: chemical composition, mineralogy, structure and properties. Applications of clays in construction and generalities in their applications in construction.
2- Plaster: chemical composition and raw material, mineralogy and manufacturing process. Properties, standards and applications.

Aluminum Cement (CAC):
- Origin and Raw Materials: Crude (dosing of crude)
- Stages of the manufacturing process: Clinkerization and formation of Clinker.
- Product monitoring techniques: FRX and DRX
- Components of calcium aluminate cement. Phase structure. Influence of anhydrous compounds or phases of clinker on their properties (reaction rate and heat, and compressive strength).
- Setting and hardening.
- Conversion or transformation of the microstructure of the aluminous cement paste.
- Durability of CAC cement
- Applications and regulations (UNE).

Regulations (UNE and RC-16), tests, limits and nomenclature.
Exercises of: - Application of Bogue. - Reasoning, choose the most suitable binder depending on the environment, ambient temperature, type of structure...etc. - Determination of the types of binders based on their chemical composition and their properties and characteristics. - Application of UNE and RC-16 regulations.

Session in the laboratory:
Session 1: determine the most appropriate consistency of the cement paste with a UNE normative test with the Vicat needle methodology.
Session 2: Mortar manufacturing and curing process.
Session 3: Analysis, calculation and determination of the strength of cement and its strength class.

Specific objectives:
Introduce to the study of the construction materials used by the Civil Engineer in his professional exercise, from the study of the conglomerating materials.
Put in context the different types of binders that characterize our Architectural Heritage. And to contextualize the evolution and advances in the binders over time to the present.
To know in depth one of the essential components of one of the most used materials in the current construction of Civil Engineering.
Knowledge of one of the cements used at the end of the first half of the 20th century. Advantages and disadvantages of its use in Civil Engineering. Knowledge of the cement used during the sixties and seventies of twentieth-century Spain.
Emphasize the need for a regulatory system in the use of different components and building materials in Civil Engineering. Know the rules of tests, rules of limits and rules of nomenclature.
Recognize the different types of binders and their applications. Assess the type of binder most suitable for the application, structure and environment.
The practical sessions encourage the active participation of students in order to be able to expand and work on the knowledge acquired in the classroom. Student learning is more powerful and meaningful, and the skills for learning skills is richer and more diverse, and more creative and divergent.

Full-or-part-time: 50h 24m
Theory classes: 16h
Practical classes: 3h
Laboratory classes: 2h
Self study : 29h 24m
**Durability**

**Description:**
- Generalities of Chemical Equilibrium (equilibrium state and equilibrium constant)
- Le Chatelier Principle
- Chemical Kinetics (reaction rate, kinetic theories, factors influencing reaction rate)
- Solved and unresolved problems about chemical equilibrium and influencing factors that affect equilibrium according to LeChateliers principle.
- Solubility of solids
- Equilibrium of solubility
- Effect of the common ion on the solubility
- Conditions for the formation or solubility of precipitates
- Solving problems to solve or to solve of:
  - Effects of the common ion in a saline environment
  - Influence of the pH in a saline solution
  - Conditions for the formation or solubilization of precipitates
- Acid-base theories
- Ionic product of water
- pH scale
- Weak acids: constant equilibrium acid and polyprotic acids
- Weak bases: constant of basic equilibrium
- Acid-base properties of saline solutions
- Calculation problems in the resolution of acid-base reactions. pH prediction in saline
- Attack processes and their consequences:
  - Solution / leaching
  - Cation exchange
  - Expansion processes (saline, sulphates and ettringite formation, Friedel's salt, alkali-aggregate reaction).

**Marine environment:**
- Definition of the 3 environments, and description of the attack by chlorides in reinforced concrete.
- Resolution and reasoning of the different processes that can affect the structures and their consequences according to the environment of affectation.
- Measures to prevent or rehabilitate structures

**Specific objectives:**
- Fundamental concept to understand chemical reactions in the durability of materials.
- Solving exercises with the aim of applying theoretical concepts to real problems.
- Theoretical knowledge to understand the action of saline, marine, pure water ... in certain building materials such as cement paste in concrete.
- Application of the theoretical concepts of solubility and / or precipitates in saline environments, acid rain, pure water ... in construction materials, mainly in hydrated cement paste.
- Theoretical concepts of acid-base reactions needed to apply it to solving real problems affecting the durability of materials.
- Be able to discern the process of attack of a saline solution and its pH and degree of aggressiveness in the process in order to assess the durability of the structure.
- Knowledge of the main attacks or processes caused mainly by the environment to building materials (metals: steels, concrete and reinforced concrete) and their consequences on the useful life or service life of the structure.
- Real problems in the structures that currently affect Civil Engineering.

**Full-or-part-time:**
- 31h 12m
- Theory classes: 7h
- Practical classes: 6h
- Self study: 18h 12m
Sustainable Development Goals (SDGs) in materials chemistry

Description:
Using the learning methodology of "Flipped Classroom" introduce the SDGs in materials chemistry the basics of:
- Responsible production.
- Modalities of sustainable consumption and production.
- Climate action.
- Take measures to combat climate change and its effects.
- Promote inclusive and sustainable industrialization and encourage innovation.
- Gender equality.

Using the "Flipped Classroom" methodology, carry out the autonomous and cooperative competence work outside the classroom (bibliographic research, scientific readings, video viewing and questionnaires (google forms and kahoots))

Specific objectives:
- Responsible production.
- Modalities of sustainable consumption and production.
- Climate action.
- Take measures to combat climate change and its effects.
- Introduction to promoting inclusive and sustainable industrialization and encouraging innovation.
- Gender equality.

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

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.

EXAMINATION RULES.

If any of the assessment activities is not carried out in the scheduled period, the grade for that activity will be compatible as zero.

They are indispensable prerequisites to pass subject and being able to realize the reevaluation exam:
1) To have carried out activity 0 that will be proposed in the classroom.
2) To have attended the laboratory practices and to have delivered the corresponding report.
BIBLIOGRAPHY

Basic:

Complementary: