

Course guide

2500009 - GECQUIMMAT - Chemistry of Materials

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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: 2023 **ECTS Credits:** 6.0 **Languages:** Catalan, English

LECTURER

Coordinating lecturer: DIEGO FERNANDO APONTE HERNÁNDEZ, SUSANA VALLS DEL BARRIO

Others: DIEGO FERNANDO APONTE HERNÁNDEZ, ANDREU CODINA MENDOZA, 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.

In order to reinforce contents, the subject also has 2 hours a week of workshop-type sessions with the aim of reviewing concepts of basic and elementary chemistry (formulation, solubility, stoichiometry, ideal gases).

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.

Although most of the sessions will be given in the language indicated, sessions supported by other occasional guest experts may be held in other languages.

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

Type	Hours	Percentage
Hours large group	30,0	20.00
Guided activities	6,0	4.00
Self study	84,0	56.00
Hours small group	6,0	4.00
Hours medium group	24,0	16.00

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, hydracidic acids, oxalic 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, hydric acids, oxalic 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

Self study : 22h 24m

Metallic materials and their durability

Description:

Classification and properties of metallic elements and metallic materials

Types of alloys: 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.

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:

Concepts and definitions: conglomerate, hydraulicity, cement paste, mortar, concrete. Setting and hardening. Building materials in Antiquity: collection of more characteristic examples.

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.

3- Lime: definitions, raw materials and classification. Lime type setting and hardening. Manufacturing, properties, standards and applications in construction.

Portland Cement: - Origin and Raw Materials: Crude (dosing of crude) - Stages of the manufacturing process: Clinkerization and formation of Clinker (baked). - Product monitoring techniques: FRX and DRX - Portland clinker components. Phase structure. Bug.

Influence of clinker compounds on their properties (reaction speed and heat, and compressive strength). - Hydration of Portland

cement: mechanisms of solubility and precipitation. Damage and hardening. Stages of the hydration process. - Analysis techniques (calorimetry and TGA) of hydration monitoring. - Structure of the hydrated cement paste: pch (microstructure). - Additions: types (puddles, fly ash, slag, silica fume, calcareous filler ...) - Addition cements and nomenclature - Other cements and special cements (nomenclature). RC-16.

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.

Carbonation attack on hydrated cement paste and its consequences on 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 qualification of the asignatura obtains from the qualifications of continuous evaluation and of the corresponding of laboratory and / or computer room. The continuous assessment consists of doing different activities, both individual and group, of an additive and formative nature, carried out during the course (inside the classroom and outside it). The qualification of teaching in the laboratory is the average of such activities. The assessment tests consist of a part with questions about concepts associated with the learning objectives of the subject in terms of knowledge or comprehension, and a set of application exercises. The qualification of the asignatura obtains from the qualifications of the continuous evaluation that corresponding:

MATERIALS CHEMISTRY EVALUATION OF CATALA-SPANISH LINE:

1- You can opt for 2 part exams or a final - global exam:

Partial exams (2 exams), E1 and E2 (80%), averaged 2 exams.

Or there is also option 1 final /global exam for the whole subject (EG 80%)

2- Classroom Activities and Tests for each Theme or Theme block (10%)

3- Teaching Practice Reports: Practices (10%).

ENDNOTE: $((E1+E2)/2) 0.80 + (\text{classroom and test-activity zero}) 0.10 + ((P1+P2)/2)0.10$.

Or:

ENDNOTE: $(EG 0.80 + (\text{classroom and test-activity zero}) 0.10 + ((PRACTICE)0.10)$.

2- Activities and proofs of the classroom of each subject or syllabus block (10%)

3- Teaching practice reports: two practices P1 and P2 (10%). FINAL NOTE: $((E1 + E2) / 2) 0.80 + (\text{classroom activities and zero test-activity}) 0.10 + ((PRACTICE) 0.10)$.

Internships will be evaluated based on mandatory and personal reports that must be submitted one week after each of the lab internship sessions.

MATERIALS CHEMISTRY EVALUATION OF ENGLISH LINE:

The evaluation of the subject by the group in English are defined by the coordinator or head of the subject, Professor Diego Aponte, which are published on the ATENEA digital campus of the subject Materials Chemistry, in English.

Laboratory practices are compulsory activities, and failure to carry out them and failure to deliver the reports results in an unsubmitted note of the general assessment of the subject. Criteria of qualification and of admission to the re-evaluation: The students suspended to the ordinary evaluation that have presented regularly in the proofs of evaluation of the asignatura suspended will have option to realize a proof of re-evaluation in the period fixed in the academic calendar. Students who have already passed it or students who have qualified as not presented will not be able to take the re-assessment test for a subject. The maximum grade in the case of taking the re-assessment exam will be five (5.0). The non-attendance of a student summoned to the re-evaluation test, held in the fixed period may not lead to the performance of another test with a later date. Extraordinary assessments will be carried out for those students who, due to accredited force majeure, have not been able to take any of the continuous assessment tests. These tests must be authorized by the corresponding head of studies, at the request of the teacher responsible for the subject, and will be carried out within the corresponding teaching period.

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 forms or test.

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