Course guide
2500207 - GECTERCIAM - Environmental Thermodynamics and Kinetics

Last modified: 01/10/2023

Unit in charge: Barcelona School of Civil Engineering
Teaching unit: 751 - DECA - Department of Civil and Environmental Engineering.

Degree: BACHELOR'S DEGREE IN ENVIRONMENTAL ENGINEERING (Syllabus 2020). (Compulsory subject).

Academic year: 2023 **ECTS Credits:** 6.0 **Languages:** Spanish

LECTURER

Coordinating lecturer: IGNACIO SEGURA PEREZ

Others: PAULA FELICIDAD RODRIGUEZ ESCALES, IGNACIO SEGURA PEREZ

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.

Generical:
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 4 hours a week of face-to-face classes in the classroom. Throughout the course, these sessions can be divided into general theoretical sessions (large group) and sessions with half the students (medium group). Medium group sessions are not taught every week and will be notified in advance by the teacher responsible for the subject.

The general theoretical classes (large group) are dedicated to the presentation of the basic concepts and materials of the subject, presentation of examples and carrying out exercises.

The mediated group sessions are dedicated to problem solving and directed activities (project work) with greater interaction with students. Practical exercises are carried out in order to consolidate the general and specific learning objectives.

Likewise, hours of work are carried out in the laboratory, which complement the theoretical sessions. These laboratory sessions allow the student to see in a practical way some of the aspects developed in the theoretical sessions, in relation to the properties and characterization of the materials most used in construction.

Support material is used in the format of a detailed teaching plan through the ATENEA virtual campus: contents, programming of evaluation and directed learning activities and bibliography.

Most of the classes will be taught in Spanish. The hours of exercises may be taught in Spanish or Catalan, as well as the practices, depending on the associate professor who collaborates at that time.

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.

LEARNING OBJECTIVES OF THE SUBJECT

Principles of Thermodynamics. Free energy and chemical potential. Thermodynamics of colloidal surfaces and systems. Balance in multicomponent systems. Ideal and non-ideal solutions. Fugacity. Adsorption. Reaction mechanisms. Reaction in solution. Environmental catalysis. Oxidation-reduction. Enzyme activity. Design of reactors. Applications.

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

Type	Hours	Percentage
Self study	90,0	60.00
Hours large group	30,0	20.00
Hours medium group	15,0	10.00
Hours small group	15,0	10.00

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:
Introduce 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: 19h 12m
Theory classes: 6h
Practical classes: 2h
Self study : 11h 12m

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.
Know Roult Law. Know the Henry constant. Gas solubility. Colligative properties.
Deepen the knowledge of the subject.

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

Exam

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

T4. Potential and activity. Thermodynamics of real solutions.

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: 14h 23m
Theory classes: 4h
Practical classes: 2h
Self study : 8h 23m

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.

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.

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

T6. Electrochemistry.

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: 12h
Theory classes: 3h
Practical classes: 2h
Self study : 7h

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: 12h
Theory classes: 3h
Practical classes: 2h
Self study : 7h

T8. Introduction to reactor design

Description:
Introduction to the design of reactors in different processes of Environmental Engineering, based on the concepts studied in the course
Problems

Full-or-part-time: 9h 36m
Theory classes: 2h
Practical classes: 2h
Self study : 5h 36m

Inverted class

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

Laboratory practices

Description:
Session in the laboratory in which some of the knowledge imparted during the course will be experimentally verified. Laboratory practices and in the computer room will be carried out

Full-or-part-time: 14h 23m
Laboratory classes: 6h
Self study : 8h 23m

GRADING SYSTEM

The qualification of the course is obtained from the continuous evaluation qualifications and the corresponding laboratory and / or computer room qualifications, and the evaluation tests

Continuous assessment consists of doing different activities, both individual and group, of an additive and formative nature, carried out during the course (within the classroom and outside of it). Specifically, the delivery of exercises is proposed at the end of each topic and the preparation of an inverted class.

The qualification of the laboratory activities is carried out based on the delivery of reports of the practices carried out in the laboratory.

The evaluation tests (2) consist of a part with questions about concepts associated with the learning objectives of the subject in terms of knowledge or understanding, and a set of application exercises.

The final grade for the course corresponds to 70% of the objective evaluation tests, 20% of the directed activities (delivery of exercises and work of the subject) and 10% of the laboratory practices.

Qualification and admission criteria for reevaluation:p Students who have been suspended in the ordinary evaluation and who have regularly taken the evaluation tests for the suspended subject will have the option of taking a reevaluation test in the period set in the academic calendar.

Attendance at practices and delivery of the laboratory report is an essential requirement for the evaluation of the subject, in ordinary or extraordinary call

Students who have already passed it or students classified as not presented will not be able to take the re-evaluation test of a subject.

The maximum grade in the case of taking the reevaluation exam will be five (5.0).

The non-attendance of a student summoned to the reevaluation test, held in the set period, may not lead to the completion of another test with a later date.Extraordinary evaluations will be carried out for those students who, due to accredited force majeure, have not been able to take any of continuous assessment tests.

These tests must be authorized by the corresponding head of studies, at the request of the professor responsible for the subject, and will be carried out within the corresponding academic period.

EXAMINATION RULES.

If any of the evaluation activities are not carried out in the scheduled period, the qualification of that activity will be reconciled as zero.

The essential requirement to be evaluated in the course is to attend the laboratory practices and have delivered the corresponding report.

BIBLIOGRAPHY

Basic:
- Atkins, P.W.; De Paula, J. Química física. 8a ed. Buenos Aires: Editorial Médica Panamericana, 2008. ISBN 9789500612487.
- Levine, I.N. Principios de fisicoquímica [on line]. 6a ed. México: McGraw-Hill, 2014 [Consultation: 24/11/2020]. Available on: http://www.ingebook.com/ib/NPcd/IB_LstBooks?cod_primaria=1000187&Sch_orden=1&Sch_todo=9786071509888. ISBN 9786071509888.

Complementary:
- Appelo C.A.J.; Postma, D. Geochemistry, groundwater and pollution. 2nd ed. Rotterdam: Balkema, 2005. ISBN 0415364213.