UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Course guides
250826 - 250826 - Reactive Transport

Last modified: 07/10/2020

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

Degree: MASTER'S DEGREE IN GEOTECHNICAL ENGINEERING (Syllabus 2015). (Optional subject).

Academic year: 2020 **ECTS Credits:** 5.0 **Languages:** Spanish, English

LECTURER

Coordinating lecturer: MAARTEN WILLEM SAALTINK

Others: ARNAU CANELLES GARCIA, MAARTEN WILLEM SAALTINK, FRANCISCO JAVIER SANCHEZ VILA

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
13310. To interpret laboratory tests and field observations so as to identify the mechanisms responsible for soil response. To propose laboratory testing programmes.
13311. To formulate and implement Finite Element and Finite Differences numerical models with the objective to analyze the processes that govern ground response, to interpret field information and to predict soil response.

Generical:
13300. To apply advanced knowledge in sciences and technology to the profesional or research practice.
13301. To lead, coordinate and develop integrated projects in Geo-Engineering.
13302. To identify and design solutions for geo-engineering problems within ethical, social and legislative frameworks.
13303. To evaluate the impact of Geo-engineering on environment, sustainable social development and the significance of working within reliable and consciensous profesional environment.
13304. To incorporate new techncologies and advanced tools in Geo-engineering into profesional and research activities.
13305. To conceive Geo-engineering as a multi-disciplinary field that includes relevant aspects from geology, sismology, hydrogeology, geotechnical and earthquake engineering, geomechanics, physics of porous media, geophysics, geomatics, natural hazard, energy and climate interactions.
13306. To promote innovation for the development of methodology, analyses and solutions in Geo-engineering
13307. To tackle and solve advanced mathematical problems in engineering from the drafting of the problem to the development of formulation and further implementation in computer programs. Particularly, to formulate, code and apply analytical and numerical advanced computational tools to project calculations in order to plan and manage them as well as to interpret results in the context of Geo-engineering and Mining engineering.

TEACHING METHODOLOGY

The course consists of theoretical classes, exercises that are made at home and then explained in class, laboratory with computer codes and an assignment that each student has to do.

LEARNING OBJECTIVES OF THE SUBJECT

To conceive soils and rocks as porous media governed by Solid and Fluid Mechanics.
To interpret laboratory tests and field observations so as to identify the mechanisms responsible for soil response. To propose laboratory testing programmes.
To formulate and implement Finite Element and Finite Differences numerical models with the objective to analyze the processes that govern ground response, to interpret field information and to predict soil response.
To analyze, discriminate and integrate geological and geotechnical information in studies and projects.
To calculate, evaluate, plan and regulate surface and groundwater resources.(Specific competence of the specialization in Groundwater Hydrology).
To assess and manage environmental impacts from waste disposal, soil contamination and groundwater pollution. (Specific competence of the specialization in Groundwater Hydrology).
To model, assess and manage geological resources, including mineral and thermal groundwater. (Specific competence of the specialization in Groundwater Hydrology).

* To know the existence of isotopes and basic isotopic techniques for hydrogeological studies.
* To distinguish stable isotopes from radioactive isotopes and the different applications derived from them.
* To Know and use the modern water dating techniques based on isotopic techniques.
* To know and use the isotopic techniques to assess the contamination and decontamination of soils and aquifers.
* To model the chemical balance and kinetic processes from the multidisciplinary point of view, incorporating thermo-hydro-geochemical concepts.
* To plan and solve in complicated cases the reactive transport equations.
* To model transport problem data in laboratory or on field.
* The basic challenges of subsoil heterogeneity and implications on predicting the transport in heterogeneous media are introduced.
* To analyze the stochastic approaches with regards to the quantification of heterogeneity-induced transport phenomena.
* To acquire the basic tools for stochastic modelling.
* To expose the modern approaches to modelling transport in heterogeneous media.

- Transport of pollutants. Advection, diffusion, dispersion, reactions of order 0 and 1. Adsorption. Transport equation. Solutions.
- Chemical reactions at equilibrium. Aqueous species activity.
- Law of mass action. Perfect and imperfect mixtures. Gases.
- Chemical Kinetics. Kinetic equations. Reaction order. Batch reactions.
- Reactive transport. Stoichiometric and matrix components. Transport equations. Solution.
- Reactive transport in columns.
- Numerical methods and modeling. Generic formulation of a numerical method. Temporal integration. Boundary Conditions. Method types. Modeling process.

STUDY LOAD

Type	Hours	Percentage
Hours medium group	9,8	7.83
Hours small group	9,8	7.83
Guided activities	6,0	4.80
Hours large group	19,5	15.59
Self study	80,0	63.95

Total learning time: 125.1 h

CONTENTS

Theory

Description:
Introduction of the transport processes (advection, dispersion and difussion) and chemical reactions (dissolution-precipitation, adsorption, speciation)
Monocomponent reactive transport equation. Notation of matrices and vectors. Stoichiometric matrix. Primary and secondary species.
Formulation of the basic reactive transport equation. Components and component matrix. Special case of half-reactions and constant activity species.
(Semi)analytical solutions for a simple binary system with an application to a fracturated medium. (Semi)analytical solutions for a complex system with an application to calcite dissolution in a coastal zone
Method of Picard and Newton-Raphson. Application of Newton-Raphson to speciation. Application of Picard and Newton-Raphson to reactive transport. Comparison between both methods
The solution of exercise 1 is given in class.
The solution of exercise 2 is given in class.

Full-or-part-time: 36h
Theory classes: 13h
Practical classes: 2h
Self study : 21h

Model codes

Description:
Explication and demo of the code Retraso
Practical use of the code Retraso to simulate bauxite formation

Full-or-part-time: 14h 23m
Practical classes: 3h
Laboratory classes: 3h
Self study : 8h 23m

Cases and systems

Description:
Diffusion in clays of reactive solutes
Equilibrium CO_2 calcite in shallow aquifers. CO_2 injection and storage in deep saline aquifers
Relation between redox and decay of organic matter. Reactive transport model of constructed wetland
Modelling the interaction between concrete and clay during 15 years in the underground laboratory of Tournemire
Thermodynamics of high salinity systems. 0D (ideally mixed) reactive transport models of saline lakes. 1D reactive transport models of saline aquifers.

Full-or-part-time: 43h 12m
Theory classes: 15h
Laboratory classes: 3h
Self study : 25h 12m

GRADING SYSTEM

The course evaluated through two exercises to be made at home and an assignment that have to be presented in class. The final mark is:
Nfin = 0.2Nex1 + 0.2Nex2 + 0.6Nass
where Nex1 is the mark of exercise 1, Nex12 is the mark of exercise 2 and where Nass is the mark of the assignments

EXAMINATION RULES.

Failure to perform a laboratory or continuous assessment activity in the scheduled period will result in a mark of zero in that activity.

BIBLIOGRAPHY

Basic:

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