Course guides
250824 - 250824 - Hydrogeochemical Modelling

Last modified: 12/12/2019

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: 2019 **ECTS Credits:** 5.0 **Languages:** Catalan, English, Spanish

LECTURER

Coordinating lecturer: MAARTEN WILLEM SAALTINK

Others: CRISTINA DOMENECH ORTI, MAARTEN WILLEM SAALTINK

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
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.
13323. To model, assess and manage geological resources, including mineral and thermal groundwater. (Specific competence of the specialization in Groundwater Hydrology).

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

El curso se divide en sesiones teóricas y problemas, donde se prevee el uso de programas convencionales de cálculo geoquímico.

LEARNING OBJECTIVES OF THE SUBJECT

To conceive soils and rocks as porous media governed by Solid and Fluid Mechanics.
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 design and execute hydraulic systems, including transportation facilities, distribution and storage of solids, liquids and gases, water treatment plants and waste management (urban, industrial or hazardous). (Specific competence of the specialization in Groundwater Hydrology).
To assess and manage projects, plants and water facilities for the environmental point of view. (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 main basic principles of multiphase contaminants flow and transportation in saturated and unsaturated areas of the subsoil.
* To understand the behaviour and transportation mechanisms of organic contaminants in non aqueous liquid phase and showing scarce solubility in water.
* To known the remediation outline for soils and aquifers and to be able to mathematically model them.
* To be able to carry on a study on the potential impact of a soil or water contamination problem on the population or the ecosystems.
* To understand the thermodynamic processes and their effect on the chemical signature of water.
* To know and model the main mass balance transfer processes.
* To understand the importance of chemical kinetics and existence of advanced geochemical models.
* To solve simple geochemical problems.

- Thermodynamics: internal energy, entropy, enthalpy, Gibbs free energy .
- Thermodynamic properties of pure substances. Equilibrium constant of a chemical reaction.
- Structure of an aqueous solution. Ionic strength. Water activity. Models of calculation of the activity coefficient of a solute.
- Acid-base: chemical acidity and alkalinity. PH control in continental waters. Neutralization capacity.
- Calculation of solution - gas - mineral equilibrium.
- Surface reactions: surface complexation model. Ion exchange.
- Redox: Relationship between potential and measured thermodynamic properties. The variable pE. pE - pH diagrams . Redox potential in natural waters. Biogeochemical cycles.
- Kinetics : elementary and totals reactions. Reaction rate. Effect of temperature.

STUDY LOAD

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

Total learning time: 125.1 h

CONTENTS

Introducción

Description:
Modelos geoquímicos: utilidad y limitaciones. Programa del curso

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

Termodinámica

Description:
Energía interna. Función de estado. Entropía. Propiedades intensivas. Potenciales termodinámicos. Entalpía. Energía libre de Gibbs. Estado estandard. Propiedades termodinámicas de substancias puras a cualquier presión y temperatura

Full-or-part-time: 7h 11m
Theory classes: 3h
Self study : 4h 11m

Termodinámica de soluciones

Description:
Propiedades termodinámicas de substancias no puras. Estado estandard de una solución. Constante de equilibrio de una reacción química. Variación con la presión y la temperatura.
Problema: Calculo del producto de solubilidad de la calcita entre 0 y 300°C y presión de vapor de agua

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

Soluciones acuosas

Description:
Estructura de una solución acuosa. Fuerza iónica. Actividad del agua. Actividad media de un soluto. Modelos de cálculo del coeficiente de actividad de un soluto. Actividad de una especie neutra.
Problema: Agua de mar

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

Complejos acuosos

Description:
Hidrólisis y potencial iónico. Complejos de esfera interna y externa. Importancia de la complejación en el cálculo de la fuerza iónica. Idem en la solubilidad de un sólido o un gas.
Problema: Solubilidad del yeso

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

Acido-base

Description:
Acidez y alcalinidad químicas. Sistema carbónico. Control del pH en las aguas continentales. Valoración de la alcalinidad. Capacidad de neutralización. Programa MEDUSA.
Problema: Distribución de especies de Al con el pH. Contaminación de un río por agua ácida.

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

Cálculo del equilibrio solución-mineral-gas

Description:
Conceptos básicos. Formulación matemática: sistemas de ecuaciones. Método iterativo de Newton-Raphson. Ejemplos de especiación y equilibrio entre fases. El programa PHREEQC.

Full-or-part-time: 7h 11m
Theory classes: 3h
Self study : 4h 11m

Cálculo de procesos

Description:
Disolución de un mineral o gas hasta equilibrio. Perturbación conocida de un componente: valoración de acidez o alcalinidad, disolución conocida de mineral o gas. Perturbación de todos los componentes: mezcla de soluciones, evaporación.

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

Reacciones de superficie

Description:
Modelo de complejación superficial. Modelos electrostáticos y no electrostáticos. Modelos empíricos. Intercambio iónico. Ejemplos: retención de Zn y As por oxidos de hierro.
Problema: Adsorción de Ni en bentonita.

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

Redox

Description:
Electrodo estándard de hidrógeno. Relación entre potencial medido y propiedades termodinámicas. La variable pE. Diagramas pE-pH. Potencial redox en aguas naturales. Ciclo biogeoquímico.
Problema: Oxidación de materia orgánica

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

Cinética

Description:
Reacciones elementales y totales. Velocidad de reacción. Efecto de la temperatura. Ejemplos de reacciones: oxidación-reducción, disolución-precipitación. Cinética versus equilibrio: hipótesis de equilibrio local.

Full-or-part-time: 7h 11m
Theory classes: 3h
Self study : 4h 11m

Cálculos geoquímicos en el Transporte Fundamentos

Description:
Procesos de transporte: difusión, advección, dispersión. Ecuación de continuidad. Acoplamiento de transporte y reacciones químicas. Resolución. Transporte reactivo con PHREEQC. Ejemplo: Desplazamiento de agua marina por agua continental.

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

GRADING SYSTEM

La evaluación se basará en la resolución de problemas.

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:
- Anderson G.M. i Crerar D.A. Thermodynamics in Geochemistry. Oxford: Oxford University Press, 1993. ISBN 019506464X.
- Nordstrom D.K. i Munoz J.L. Geochemical Thermodynamics. 2nd ed. Boston: Blackwell Scientific, 1994. ISBN 0865422745.
- Galí, S. Termodinámica aplicada a la geologia. Barcelona: Edicions Universitat de Barcelona, 1999. ISBN 8483381001.
- Appelo C.A.J.; Postma, D. Geochemistry, groundwater and pollution. 2nd ed. Rotterdam: Balkema, 2005. ISBN 0415364213.
- Morel, F.M.M.; Hering, J.G. Principles and applications of aquatic chemistry. New York [etc.]: Wiley, 1993. ISBN 0471548960.
- Langmuir, D. Aqueous environmental geochemistry. Upper Saddle River (N.J.): Prentice Hall, 1997. ISBN 0023674121.
- Stumm W. i Morgan J.J. Aquatic chemistry. 3a ed. New York: John Wiley and Sons, 1996. ISBN 0471511854.