Pollutant Transport Modelling (250MEA011)

General Information

School	ETSECCPB
Departments	Departament d'Enginyeria Civil i Ambiental (DECA)
Credits	5.0 ECTS
Programs	MÀSTER UNIVERSITARI EN ENGINYERIA AMBIENTAL (pla 2024) MÀSTER UNIVERSITARI EN ENGINYERIA DE L'AIGUA (pla 2025)
Course	2025/26

Main teaching language at each group

- Group 10Q2 Spanish (Q2)

Faculty

Responsible Faculty: Daniel Fernandez Garcia
Faculty: Daniel Fernandez Garcia, Guillem Solé Marí

Objectives of Education

Know how to solve environmental problems using numerical methods with the application of theoretical concepts of flow and contaminant transport in the natural environment.
Learn to formulate and program numerical models using Finite Elements and Finite Differences to analyze the processes that govern the response of the natural environment, interpret field information, and predict the response of the environment.

General process of modeling natural phenomena.
Basic formulation of problems of flow and contaminant transport.
Formulation of the flow equation.
Solution of the flow equation using numerical methods.
Methodology for modeling flow in aquifers.
Formulation of the transport equation.
Inverse problem and calibration.
Numerical solution of the transport equation and its difficulties.
Real cases.

Total hours of student work

		Hours	Percentage
Supervised Learning	Large group	35.0 h	77.78 %
	Medium group	0.0 h	0.00 %
	Laboratory classes	10.0 h	22.22 %
	Guided Activities	0.0 h	0.00 %
Self Study		80.0 h	

Contents

Introduction

What is a model? Types. Utility. Difficulties. The modeling process
A generic numerical method. Application to solving the flow equation. Typical program structure. Review of the most used numerical methods and comparison of them. The modeling process. Conceptual model. Boundary and initial conditions. Calibration and validation
Illustration example.

Solution of the flow equation through Finite Diferences

General formulation eq. Flow (Review)
Finite difference scheme. Formal derivation
Temporal integration methods. Implicit, explicit, and Crank-Nicholson schemes. Boundary conditions. Types and implementation.
Stability. Consistency and truncation error. Convergence and convergence error
Solution of the linear system of equations

Solution of the flow equation using the finite element method

Generalities. Weighted residuals. Alternative formulations
Finite elements. Discretization and shape functions. Derivation of equations by the Galerkin method.
Other types of elements. Simple, complex, multiple, isoparametric. Application to the simple 2D case.
Temporal integration schemes.
Application to a one-dimensional case.

Solution of the transport equation using classical Eulerian methods

Mechanisms of solute transport. Basic formulations
Finite differences. Integrated finite differences. Upstream weighting
Finite elements
Discussion of stability issues. Conditions on the Peclet and Courant numbers
Application to a one-dimensional case.

title englishSolution of the transport equation using lagrangian approaches

Purely Lagrangian methods. Evaluation of the material derivative. Limitations
Eulerian-Lagrangian methods. Particle methods
Random walk method
Comparison between different methods.

Solution of the inverse problem and automatic calibration

Automatic calibration versus manual calibration
Linear and nonlinear regression, sensitivity matrix
Calibration statistics

Solution of nonlinear problems of flow and transport

Generalities. Newton-Raphson method, Picard,…
Solution of the flow eq. for free aquifer. Example
Unsaturated medium. Example
Reactive Transport. Example

Workshops

Learning MODEL MUSE

Activities

Performing a case study

Dedication

10h

Teaching Methodology

The course consists of 3 hours a week of classes in a classroom.
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 hour is devoted to solving practical problems with greater interaction with the students. The objective of these practical work and exercises is to consolidate the general and specific learning objectives.
Support material in the form of detailed teaching plan is used by: content, program of learning and assessment activities conducted and literature.

Grading Rules

(*) The evaluation calendar and grading rules will be approved before the start of the course.

The course grade will be obtained from continuous assessment scores and corresponding practical work.
Continuous assessment consists in several activities, both individually and in group, of additive and formative characteristics, carried out during the course (in the classroom and beyond).
The evaluation tests consist of a part with basic issues and questions about concepts associated with the learning objectives of the course with in terms of knowledge or understanding concepts, and a set of exercises for understanding and application.
The teaching takes place according to the following criteria:
NF = r*NE +(1-r)*NAC, r = 0,8
NAC = q*NAEP +(1-q)*NACET, q = 0,8

NF: Final Note
NE: Exam Note
NAC: Note from continuous assessment
NAEP: Note teachings practical assessment (works, presentations, etc.)
NACET: Note continued evaluation of the theoretical teachings (test, etc.)

Test Rules

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

Office Hours

Constantly available via email:
daniel.fernandez.g@upc.edu

Bibliography

Basic

- Zheng, C. Applied contaminant transport modeling: theory and practice. New York: Van Nostrand Reinhold, 1995. ISBN 0442013485.
- Anderson, M.P.; Woessner, W.W.; Hunt, R.J. Applied groundwater modeling: simulation of flow and advective transport. 2nd ed. Amsterdam, [Netherlands]: Academic Press, 2015. ISBN 9780080916385.
- Harbaugh, A.W.; Banta, E.R.; Hill, M.C.; McDonald, M.G. MODFLOW-2000: the U.S. Geological Survey Modular Ground-Water Model: user guide to modularization concepts and the ground-water flow process. U.S. Geological Survey, 2000.
- Istok, J. Groundwater modeling by the finite element method. Washington: American Geophysical Union, 1989. ISBN 0875903177.
- Pinder, G.F.; Gray, W.G. Finite element simulation in surface and subsurface hydrology. San Diego: Academic Press, 1977. ISBN 0125569505.