# Course guide
# 250MEA011 - 250MEA011 - Pollutant Transport Modelling

**Last modified:** 15/06/2025

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

**Degree:** MASTER'S DEGREE IN ENVIRONMENTAL ENGINEERING (Syllabus 2024). (Optional subject).
MASTER'S DEGREE IN WATER ENGINEERING (Syllabus 2025). (Optional subject).

**Academic year:** 2025 **ECTS Credits:** 5.0 **Languages:** Spanish

## LECTURER

**Coordinating lecturer:** DANIEL FERNANDEZ GARCIA

**Others:** MAARTEN W. SAALTINK
Solé Marí, Guillem

## 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.

## LEARNING OBJECTIVES OF THE SUBJECT

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.

## STUDY LOAD

| Type | Hours | Percentage |
|---|---|---|
| Self study | 80,0 | 64.00 |
| Hours large group | 35,0 | 28.00 |
| Hours small group | 10,0 | 8.00 |

**Total learning time:** 125 h

## CONTENTS

### Introduction

**Description:**
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.

**Full-or-part-time:** 2h
Theory classes: 2h

### Solution of the flow equation through Finite Diferences

**Description:**
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

**Full-or-part-time:** 6h
Theory classes: 6h

### Solution of the flow equation using the finite element method

**Description:**
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.

**Full-or-part-time:** 6h
Theory classes: 6h

### Solution of the transport equation using classical Eulerian methods

**Description:**
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.

**Full-or-part-time:** 6h
Theory classes: 6h

### title englishSolution of the transport equation using lagrangian approaches

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

**Full-or-part-time:** 4h
Theory classes: 4h

### Solution of the inverse problem and automatic calibration

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

**Full-or-part-time:** 4h
Theory classes: 4h

### Solution of nonlinear problems of flow and transport

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

**Full-or-part-time:** 3h
Theory classes: 3h

### Workshops

**Description:**
Learning MODEL MUSE

**Full-or-part-time:** 8h
Theory classes: 8h

## GRADING SYSTEM

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.)

## EXAMINATION 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.

## 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 [on line]. 2nd ed. Amsterdam, [Netherlands]: Academic Press, 2015 [Consultation: 04/10/2024]. Available on: https://web-p-ebscohost-com.recursos.biblioteca.upc.edu/plink?key=100.65.189.54_8000_228321815&AN=1037869&site=ehost-live&db=nlebk&scope=site. 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 [on line]. U.S. Geological Survey, 2000 [Consultation: 17/09/2024]. Available on: https://pubs.usgs.gov/publication/ofr200092.
- 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.

## RESOURCES

**Computer material:**
- MODEL MUSE. ModelMuse is a graphical user interface (GUI) developed by the U.S. Geological Survey for building and running groundwater models using MODFLOW and other related software. It allows users to create and visualize model grids, input parameters, and boundary conditions interactively. ModelMuse supports the design and simulation of complex groundwater flow and transport processes, providing a user-friendly environment for researchers and practitioners in hydrogeology.