Universitat Autònoma de Barcelona

2023/2024

Computational Fluid Dynamics and Process Optimisation

Code: 43325
ECTS Credits: 9

Degree	Type	Year	Semester
4314579 Biological and Environmental Engineering	OB	1	A

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Teachers

Albert Guisasola Canudas

External teachers

Martí Cortada García

Prerequisites

Mass and energy balances.
Transport phenomena.
Chemical and biological kinetics.
Differential calculation. Ordinary differential equations. Differential equations with partial derivatives.
Numerical methods.
Programming languages. Matlab.

Basic skills in technical drawing using software AutoCAD-type

Objectives and Contextualisation

The main objective is twofold, on the one hand the application with criteria of tools for modelling, simulation and optimisation of chemical, biotechnological and environmental processes and, on the other hand, to work on the bases of Computational Fluid Dynamics.
The specific objectives of the course are:
- Formulate mathematical models for different processes from non-stationary state balances and other additional equations.

- Numerically solve mathematical models with simulation programs and analyze the results.
- Use methods for univariate and multivariate mathematical optimization.
- Adjust mathematical models. Analyze the sensitivity of model parameters.
- Apply the basic notions of experimental design.
- Develop calculation programs, based on the fundamental principles of Transport Phenomena and the appropriate Numerical Methods.
- To solve problems of Transport Phenomena in such a way that the student can understand how they are structured and which are the principles of operation of the commercial CFD packages, mainly ANSYS

Learning Outcomes

- CA09 (Competence) Integrate knowledge of kinetics, thermodynamics, transport phenomena and numerical methods to analyse, design, model and optimise different types of reactors and their operating strategies.
- CA09 (Competence) Integrate knowledge of kinetics, thermodynamics, transport phenomena and numerical methods to analyse, design, model and optimise different types of reactors and their operating strategies.
- CA10 (Competence) Formulate and solve univariate and multivariate mathematical and technical-economic optimisation problems.
- KA06 (Knowledge) Recognise the structure and use of commercial Computational Fluid Dynamics (CFD) packages.
- KA07 (Knowledge) Define the basic notions of experimental design.
- SA06 (Skill) Deduce the learning skills required to continue one's training in a self-managed or autonomous manner.
- SA06 (Skill) Deduce the learning skills required to continue one's training in a self-managed or autonomous manner.
- SA07 (Skill) Build mathematical models of processes in a steady or non-steady state using suitable numerical methods to solve these models.
- SA08 (Skill) Deduce the equations of change of Transport Phenomena to solve engineering problems in order to establish the model for a system.
- SA09 (Skill) Use the most adequate IT instruments to complement knowledge in the field of biological engineering and environmental engineering.
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Content

The subject is structured in two modules:

Modeling and optimization of processes
- Modelling of chemical, biological and environmental processes
- Simulation of processes with ordinary differential equations
- Simulation of processes with differential equations with contour conditions
- Simulation of processes with differential equations with partial derivatives
- Univariate, multivariate and constrained optimization methods
- Model fit: Parameter Determination and Sensitivity Analysis
- Design of experiments

Computational Fluid Dynamics
- Introduction
- Geometry and mesh
- The integrator
- The Visualizer

- Case Studies

Methodology

The course will be developed in theory classes and theoretical-practical classes. In addition, during the course different proposed cases will have to be solved and presented, which will be carried out mainly outside the class schedule.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Theoretical and theoretical-practical classes	56	2.24	CA09, CA10, KA06, KA07, SA07, SA08, SA09, CA09
Type: Supervised			
Approach to the resolution of proposed cases	14	0.56	CA09, CA10, KA06, SA06, SA07, SA08, SA09, CA09
Type: Autonomous			
Study, search for information and resolution of the proposed cases.	89	3.56	CA09, KA06, KA07, SA06, SA08, SA09, CA09

Assessment

Evaluation

(a) Scheduled evaluation process and activities

The course is divided into two independent modules: 1) Computational Fluid Dynamics (CFD) and 2) Process Modeling and Optimization (MOP).
Below are the evaluation activities of each module of the subject with its percentage of weight on the final grade:

Process Modeling and Optimization
- Activity 1 (15%). Problems
- Activity 2 (60%). Partial exam
- Activity 3 (25%). Modelling work on real scientific papers.

Computational Fluid Dynamics

- Activity 1 (5%). Course work CFD1.

- Activity 2 (10%). Course work CFD2.

- Activity 3 (15%). Course work CFD3.

- Activity 4 (70%). Exam.

The final grade is the average grade of the two modules. The grade for each module must be greater than or equal to 4.5/10 in order to make the average.You need at least a 3.0/10 in each of the exams to pass the module.
The non-presence in class when evaluation tests are carried out is a zero of the activity, without possibility of recovery.

b) Programming of evaluation activities

The schedule of evaluation activities will be given on the first day of the course and will be made public through the Moodle.

c) Recovery process

Student can apply for make-up of each module as long as they have presented himself to a set of activities that represent at least two thirds of the total grade of the module. Of these, those students who have a grade of more than 3.0 on average for all the activities in the module may be presented for make-up.
The make-up process of each module will consist of an exam with all the contents of the module. The maximum grade that can be obtained using this procedure will be 6.0 in each module recovered.

d) Procedure for revision of qualifications

For each assessment activity, a place, date and time of review will be indicated where the student can review the activitywith the professor. In this context, complaints can be made about thegrade of the activity, which will be evaluated by the professor responsible for the subject. If the student does not submit to this review, this activity will not be reviewed at a later date.

e) Qualifications

In case one of the modules does not reach 4.5/10, the maximum final grade of the course will be 4/10 and the suspended module will have to be repeated the following year.

Honour plates. It is the decision of the faculty responsible for the subject to award an honorary matriculation grade. UAB regulations state that MH can only be awarded to students who have obtained a final grade equal to or higher than 9.00. Up to 5% of the total number of students enrolled may be awarded.

A student will be considered non-assessable (NE) if he/she has not presented to a set of activities whose weight equals a minimum of two thirds of the total grade of the subject.

f) Student Irregularities, Copying and Plagiarism

Without prejudice to other disciplinary measures that may be deemed appropriate, irregularities committed by the student that may lead to a variation in the grade of an evaluation act shall be graded with a zero. Therefore, copying, plagiarism, cheating, letting copy, etc. in any of the evaluation activities will involve suspending it with a zero. Evaluation activities graded in this way and by this procedure will not be recoverable.

h) Evaluation of Repeating Students

The only change in subject evaluation for repeaters is the possibility of maintaining grades from a module passed the previous course. This option must be communicated by email to the teacher responsible, no later than 15 days after the start of classes.

SINGLE ASSESSMENT
This course does not offer a single assessment

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
CFD. Case study resolution	15	30	1.2	CA09, KA06, KA07, SA06, SA09
CFD. Exam	35	3	0.12	CA09, KA06, KA07, SA09
MOP. Exam	30	3	0.12	CA09, CA10, KA07, SA06, SA07, SA08, SA09
MOP. Problem delivery.	7.5	10	0.4	CA09, CA10, KA07, SA06, SA07, SA08, SA09
MOP. Work/s of modelling and simulation of real systems	12.5	20	0.8	CA09, CA10, KA07, SA06, SA07, SA08, SA09

Bibliography

- J.D. Anderson. Computational Fluid Dynamics. The basics with Applications. McGraw-Hill, Inc., 1995.

- H.K. Versteeg, W. Malalasekera. An Introduction to Computational Fluid Dynamics. The Finite Volume Method. Prentice Hall, 2nd ed., 2007.

- S.V. Patankar, "Numerical Heat transfer and Fluid Flow". Hemisphere Pub., 1980.

- J. Tu, G.H. Yeoh, C. Liu. Computational Fluid Dynamics. A practical Approach. Elsevier, 2nd ed., 2013

- Jiyuan Tu, Guan-Heng Yeoh and Chaoqun Liu. Computational Fluid Dynamics: A Practical Approach, 2008.

- R. Byron Bird, Warren E. Stewart, Edwin N. Lightfoot. Transport Phenomena, 2002.

- Blazek J. Computational Fluid Dynamics: Principles and applications, 2005.

- Ferziger J., Peric M. Computational Method for Fluid dynamics, 2020

- B.W. Bequette. Process Dynamics. Modeling Analysis and Simulation. Prentice-Hall. International Series in the Physical and Chemical Engineering Sciences, 1998.

- W.L. Luyben. Process Modeling, Simulation and Control for Chemical Engineers, 2nd ed. McGraw-Hill, New York, 1990.

- MATLAB. The MathWorks MATLAB® http://es.mathworks.com/ Versión estudiante: MATLAB & Simulink Student Version. https://es.mathworks.com/programs/nrd/buy-matlab-student.html

- Yeong Koo Yeo;Yeong Koo Yeo. Chemical Engineering Computation with MATLAB® 2020

- Al-Malah K MATLAB Numerical Methods with Chemical Engineering Applications, 2013

Software

A minimum level of MATLAB is required to undertake the course. The CFD part will be taught in FLUENT