2020/2021

Computational Fluid Dynamics and Process Optimisation

Code: 43325
ECTS Credits: 9

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

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

Contact

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Use of Languages

Principal working language: spanish (spa)

Other comments on languages

50 % of the subject will be in English

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

Competences

- Apply specific methodologies, techniques and resources to conduct research and produce innovative results in the area of biological and environmental engineering.
- Continue the learning process, to a large extent autonomously.
- Integrate knowledge and use it to make judgements in complex situations, with incomplete information, while keeping in mind social and ethical responsibilities.
- Integrate knowledge of kinetics, thermodynamics, transport phenomena and numerical methods to analyse, design, model and optimise different types of biological reactors and their operating strategy.
- Solve problems in new or little-known situations within broader (or multidisciplinary) contexts related to the field of study.
- Use IT tools to acquire further knowledge in the field of biological and environmental engineering.
- Use acquired knowledge as a basis for originality in the application of ideas, often in a research context.

Learning Outcomes

1. Analyse the structure and workings of CFD commercial packages.
2. Apply change equations of transport phenomena to engineering-problem solving to set up the model of the system.
3. Apply specific methodologies, techniques and resources to conduct research and produce innovative results in the area of biological and environmental engineering.
4. Construct mathematical models of steady- and unsteady-state chemical processes.
5. Continue the learning process, to a large extent autonomously.
6. Define, formulate and solve technical-economic optimisation problems.
7. Develop calculation programmes to solve equations of transport phenomena in specific problems.
8. Integrate knowledge and use it to make judgements in complex situations, with incomplete information, while keeping in mind social and ethical responsibilities.
9. Interpret change equations of transport phenomena on the basis of the physical principles that govern them.
10. Solve problems in new or little-known situations within broader (or multidisciplinary) contexts related to the field of study.
11. Use IT tools to acquire further knowledge in the field of biological and environmental engineering.
12. Use acquired knowledge as a basis for originality in the application of ideas, often in a research context.
13. Use and programme appropriate numerical methods to resolve models.
14. Use simulation to assess and predict the behaviour of systems.

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.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Theoretical and theoretical-practical classes	56	2.24	1, 2, 4, 6, 9, 12, 13, 14
Type: Supervised			
Approach to the resolution of proposed cases	14	0.56	8, 10, 5, 12
Type: Autonomous			
Study, search for information and resolution of the proposed cases.	89	3.56	1, 3, 2, 4, 6, 7, 9, 8, 10, 5, 12, 13, 14, 11

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 (20%). Problems
- Activity 2 (40%). Partial exam
- Activity 3 (40%). Modelling work on real scientific papers.

Computational Fluid Dynamics

- Activity 1 (10%). Course work CFD1.

- Activity 2 (20%). Course work CFD2.

- Activity 3 (30%). Course work CFD3.

- Activity 4 (40%). Exam.

The final grade is the average grade of the two modules. The grade for each module must be greater than or equal to 5/10 in order to make the average.
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 activity with 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 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.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes

CFD. Case study resolution	30	30	1.2	1, 2, 7, 9, 8, 10, 5, 12, 13, 14
CFD. Exam	20	3	0.12	1, 2, 7, 9, 8, 10, 5, 12, 13, 14
MOP. Exam	15%	3	0.12	4, 6, 8, 10, 5, 12, 13, 14
MOP. Problem delivery.	10%	10	0.4	3, 4, 6, 8, 10, 5, 12, 13, 14, 11
MOP. Work/s of modelling and simulation of real systems	25%	20	0.8	3, 4, 6, 8, 10, 5, 12, 13, 14, 11

Bibliography

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