



# Course guide

## 295563 - 295EQ141 - Computational Fluid Dynamics

Last modified: 14/06/2023

**Unit in charge:** Barcelona East School of Engineering  
**Teaching unit:** 713 - EQ - Department of Chemical Engineering.

**Degree:** MASTER'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2019). (Optional subject).

**Academic year:** 2023    **ECTS Credits:** 6.0    **Languages:** English

### LECTURER

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**Coordinating lecturer:** Planas Cuchi, Eulalia

**Others:**

### PRIOR SKILLS

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Transport Phenomena, programming

### DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

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#### Generical:

CGMUEQ-01. Ability to apply the scientific method and the principles of engineering and economics, to formulate and solve complex problems in processes, equipment, facilities and services, in which the matter undergoes changes in its composition, state or energy content, characteristic of the chemical industry and other related sectors among which are the pharmaceutical, biotechnological, materials, energy, food or environmental

CGMUEQ-04. To carry out the appropriate research, undertake the design and manage the development of engineering solutions, in new or little known environments, relating creativity, originality, innovation and technology transfer

CGMUEQ-05. Know how to establish mathematical models and develop them through appropriate information technology, as a scientific and technological base for the design of new products, processes, systems and services, and for the optimization of others already developed

#### Transversal:

05 TEQ. TEAMWORK. Being able to work as a team player, either as a member or as a leader. Contributing to projects pragmatically and responsibly, by reaching commitments in accordance to the resources that are available.

03 TLG. THIRD LANGUAGE. Learning a third language, preferably English, to a degree of oral and written fluency that fits in with the future needs of the graduates of each course.

### TEACHING METHODOLOGY

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- Regular classes
- Hands-on workshops
- Project based learning
- Seminars

### LEARNING OBJECTIVES OF THE SUBJECT

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After this course the students should be able to do CFD analysis correctly but not to write their own CFD code. They should also be able to understand the strengths and weaknesses of CFD simulations, and apply it to solve advanced problems involving turbulence modelling, mixing, reaction/combustion and multiphase flows.



## STUDY LOAD

Type	Hours	Percentage
Hours large group	28,0	18.67
Hours small group	14,0	9.33
Guided activities	6,0	4.00
Self study	102,0	68.00

**Total learning time:** 150 h

## CONTENTS

### 1- GENERAL INTRODUCTION TO CFD MODELLING

**Description:**

- Modelling in engineering
- CFD simulations
- Applications in engineering
- Types of flow

**Specific objectives:**

To explain the input needed to solve CFD problems (CAD geometry, computational mesh, material properties, boundary conditions...), to discuss briefly the difficulty and accuracy of CFD simulations for various applications

**Full-or-part-time:** 5h 30m

Theory classes: 1h 30m

Self study : 4h

### 2- CFD SOFTWARES

**Description:**

- General purpose CFD programs available
- FLUENT
- FDS
- OPENFOAM

**Specific objectives:**

To introduce the most used commercial CFD programs available, to provide a general view of the three tools that will be used during the course: Fluent, FDS and OpenFOAM.

**Related activities:**

FLUENT, FDS and OpenFOAM tutorials to do at home.

**Full-or-part-time:** 9h 30m

Theory classes: 1h 30m

Self study : 8h

### 3- MODELLING

**Description:**

- Mass, heat and momentum balances
- The equation of continuity
- The equation of motion
- Energy transport
- The balance for species
- Boundary conditions
- Physical properties

**Specific objectives:**

To provide an overview of the equations that are the basis of the CFD modelling and the parameters needed to solve them.

**Related activities:**

**Full-or-part-time:** 5h 30m

Theory classes: 1h 30m

Self study : 4h

### 4- NUMERICAL ASPECTS OF CFD TOOLS

**Description:**

- Numerical methods for CFD
- Cell balancing
- The Gauss-Seidel algorithm
- Measures of convergence
- Discretization schemes
- Solving the velocity field
- Unsteady flows
- Meshing

**Specific objectives:**

To introduce commonly used numerical methods. To explain the various methods so that the student will be able to choose the appropriate method with which to perform CFD simulations.

**Related activities:**

Laboratory session 1: Numerical methods

Laboratory session 2: The velocity field

Laboratory session 3: Cell balancing and meshing

**Full-or-part-time:** 27h 30m

Theory classes: 3h

Laboratory classes: 4h 30m

Self study : 20h



## 5- TURBULENT FLOW MODELLING

### Description:

- The physics of fluid turbulence
- Turbulence modelling
- Near-wall modelling
- Inlet and outlet boundary conditions

### Specific objectives:

To provide an insight into the physical nature of turbulence and the mathematical framework that is used in numerical simulations of turbulent flows. To explain why turbulence must be modelled and how turbulence can be modelled.

### Related activities:

Laboratory session 4: Turbulence modelling  
Laboratory session 5: Boundary conditions  
Laboratory session 6: Project – Problem definition  
Laboratory session 7: Project – Technical data  
Laboratory session 8: Project - Geometry

**Full-or-part-time:** 47h 30m

Theory classes: 6h

Laboratory classes: 7h 30m

Self study : 34h

## 6- TURBULENT MIXING, CHEMICAL REACTIONS AND MULTIPHASE FLOW MODELLING

### Description:

- Problem description
- The nature of turbulent mixing
- Mixing of a conserved scalar
- Modelling of chemical reactions
- Non-PDF models
- Multiphase flow modelling

### Specific objectives:

To give an introduction to problems faced by engineers wanting to use CFD for detailed modelling of turbulent reactive flows and of multiphase flows. To describe the physical processes of turbulent mixing and know why this can have an effect on the outcome of chemical reactions.

### Related activities:

Laboratory session 9: Project – Mesh analysis  
Laboratory session 10: Project – Simulations 1  
Laboratory session 11: Projects – Simulations 2  
Laboratory session 12: Project - Results  
Laboratory session 13: Project - Report

**Full-or-part-time:** 47h 30m

Theory classes: 6h

Laboratory classes: 7h 30m

Self study : 34h



## 7- BEST PRACTICES GUIDELINES

### Description:

- Application uncertainty
- Numerical uncertainty
- Numerical errors
- Turbulence modelling
- Reactions and multiphase modelling
- Sensitivity analysis
- Verification, validation and calibration

### Related activities:

To understand the limitations of the CFD modelling, to explain most common sources of errors and to provide best practices guidelines for CFD simulations.

### Full-or-part-time: 7h

Theory classes: 1h 30m

Laboratory classes: 1h 30m

Self study : 4h

## GRADING SYSTEM

$$NF = 0,4 * NEF + 0,3* NEP + 0,3 * NP$$

NF : Final grade

NEF: Final exam grade

NEP = Mean grade of the practical exercises

NP: Project's grade

## EXAMINATION RULES.

The tests can be done with all the material that the student needs.

## BIBLIOGRAPHY

### Basic:

- Anderson, B. Computational fluid dynamics for engineers. Cambridge University Press, 2012. ISBN 9781107018952.

### Complementary:

- Fox, Rodney O. Computational models for turbulent reacting flows. Cambridge: Cambridge University Press, 2003. ISBN 9780521659079.

- Kolev, Nikolay Ivanov. Multiphase flow dynamics [on line]. 2nd ed. Berlin [etc.]: Springer Science & Business Media, 2005 [Consultation: 12/05/2020]. Available on: <https://link.springer.com/book/10.1007/b138144>. ISBN 3540268294.

- Davidson, Peter. Turbulence : an introduction for scientists and engineers. 2nd ed. Oxford: Oxford University Press, [2015]. ISBN 9780198722595.

- Yeoh, Guan Heng; Yuen, Kwok Kit (eds.). Computational fluid dynamics in fire engineering : theory, modelling and practice. Amsterdam ; Boston: Elsevier, 2009. ISBN 9780750685894.

- Schlichting (Deceased), Hermann; Gersten, Klaus. Boundary-Layer theory [on line]. 9th ed. Berlin, Heidelberg: Springer, 2017 [Consultation: 12/05/2020]. Available on: <http://dx.doi.org/10.1007/978-3-662-52919-5>. ISBN 9783662529195.