Course guides
295563 - 295EQ141 - Computational Fluid Dynamics

Last modified: 09/07/2021

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: 2021 **ECTS Credits:** 6.0 **Languages:** English

LECTURER

Coordinating lecturer: Planas Cuchi, Eulalia

Others: Pastor Ferrer, Elsa
Guardo Zabaleta, Alfredo
Águeda Costafreda, Alba

PRIOR SKILLS

Transport Phenomena, programming

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

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

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

LEARNING OBJECTIVES OF THE SUBJECT

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
Guided activities	6,0	4.00
Hours large group	28,0	18.67
Hours small group	14,0	9.33
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.