Course guide
295563 - 295EQ141 - Computational Fluid Dynamics

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: 2022 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

<table>
<thead>
<tr>
<th>Type</th>
<th>Hours</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Guided activities</td>
<td>6.0</td>
<td>4.00</td>
</tr>
<tr>
<td>Hours large group</td>
<td>28.0</td>
<td>18.67</td>
</tr>
<tr>
<td>Hours small group</td>
<td>14.0</td>
<td>9.33</td>
</tr>
<tr>
<td>Self study</td>
<td>102.0</td>
<td>68.00</td>
</tr>
</tbody>
</table>

**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

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**GRADING SYSTEM**

\[ NF = 0.4 \times NEF + 0.3 \times NEP + 0.3 \times NP \]

- **NF**: Final grade
- **NEF**: Final exam grade
- **NEP**: Mean grade of the practical exercises
- **NP**: Project's grade

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**EXAMINATION RULES.**

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

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**BIBLIOGRAPHY**

**Basic:**

**Complementary:**