Zał. nr 5 do ZW 78/2023

Attachment no. 4. to the Program of Studies

FACULTY of Chemistry

**SUBJECT CARD**

**Name of subject in Polish** Projektowanie procesów chemicznych z użyciem obliczeń CFD
**Name of subject in English** Chemical Process Project with CFD calculations
**Main field of study (if applicable):** Chemical Engineering and Technology
**Specialization (if applicable):** Advanced Chemical Engineering
**Profile: academic ~~/ practical~~***
**Level and form of studies: ~~1st/~~ 2nd level, ~~uniform magister studies~~*, full-time ~~/ part-time~~***
**Kind of subject: obligatory ~~/ optional / university-wide~~***
**Subject code W03CET-SM2006W, W03CET-SM2006P**
**Group of courses ~~YES~~ / NO***

| | Lecture | Classes | Laboratory | Project | Seminar |
|---|---|---|---|---|---|
| Number of hours of organized classes in University (ZZU) | 15 | | | 60 | |
| Number of hours of total student workload (CNPS) | 50 | | | 100 | |
| Form of crediting (Examination / crediting with grade) | crediting with grade | | | crediting with grade | |
| For group of courses mark (X) final course | | | | | |
| Number of ECTS points | 2 | | | 4 | |
| including number of ECTS points for practical classes (P) | | | | 4 | |
| including number of ECTS points corresponding to classes that require direct participation of lecturers and other academics (BU) | 0.6 | | | 2,4 | |

*delete as not necessary

**PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES**

1. Knowledge of mathematics at a level that allows to understand the transport equations in single- and multi-phase systems, with laminar and turbulent flow
2. Knowledge of the fundamentals of momentum, heat and mass transfer in chemical devices

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**SUBJECT OBJECTIVES**

C1. Acquainting students with the basics of CFD methods and their areas of application
C2. Acquire basic skills to perform CFD calculations of momentum, heat and mass transfer in laminar and turbulent flow, in single and multiphase, steady and transient systems, with the help of a selected software package
C3. Acquiring basic skills in the design and optimization of apparatus construction used in the chemical industry using CFD methods
C4. Familiarization with modern programs for simulation and design of chemical installations
C5. Teaching how to perform simulation calculations and design of chemical installations
C6. Teaching how to search and process calculation results

**SUBJECT EDUCATIONAL EFFECTS**

relating to knowledge:
PEU_W01 - knows the principles of building mathematical models of processes and solving them using CFD methods
relating to skills:

PEU_U01 - can build a mathematical model of the process and perform simulation calculations using specialized software
PEU_U02 - is able to perform design calculations of selected unit operations with the use of specialized software
relating to social competences:
PEU_K01 - can work in a group

## PROGRAMME CONTENT

| Lecture | | Number of hours |
|---|---|---|
| Lec1 | Familiarization with the basics of CFD methods, their advantages and disadvantages, area of application | 1 |
| Lec2 | Presentation of the equations of momentum, heat and mass transport of a Newtonian fluid for laminar one phase flow. | 1 |
| Lec3 | Definition of turbulence, different approaches to the description of turbulent flows | 1 |
| Lec4 | Presentation of turbulence models | 1 |
| Lec5 | Different ways of describing the boundary zone | 1 |
| Lec6 | Presentation of numerical basics of methods for solving momentum, heat and mass transport equations (difference and finite element methods, control volume method) | 1 |
| Lec7 | Interpolation Schemes and pressure calculation | 1 |
| Lec8 | Description of boundary conditions | 1 |
| Lec9 | Numerical mesh (different types and ways of generation) | 1 |
| Lec10 | Methods for evaluating and improving the quality of the numerical mesh | 1 |
| Lec11 | General classification of multiphase models | 1 |
| Lec12 | VOF and Level Set models | 1 |
| Lec13 | Euler-Euler and Euler-Lagrange models | 1 |
| Lec14 | Selection of a multiphase model | 1 |
| Lec15 | Selection of the right computer hardware for CFD calculations | 1 |
| | Total hours | **15** |
| **Project** | | **Number of hours** |
| Pr1 | Introduction. Flash simulation. | 2 |
| Pr2 | Distillation process simulation | 2 |
| Pr3 | Sensitivity analysis | 2 |
| Pr4 | Design specification | 2 |
| Pr5 | Physical property analysis | 2 |
| Pr6 | Physical property estimation | 2 |
| Pr7 | Detailed design of heat exchanger | 2 |
| Pr8 | Test I | 2 |
| Pr9 | Chemical reactor simulation | 2 |
| Pr10 | Chemical plant optimization | 2 |

| | | |
|---|---|---|
| Pr11 | Design of distillation column | 2 |
| Pr12 | Parameter regression | 2 |
| Pr13 | Analysis of heat exchanger network | 2 |
| Pr14 | Synthesis of heat exchanger network | 2 |
| Pr15 | Test II | 2 |
| Pr16 | Basic information about the CFD package user interface, navigating in the program, solving a simple laminar flow example in a pipe, creating simple geometry, generating a mesh, defining boundary conditions | 2 |
| Pr17 | Simulation of a single-phase laminar flow in different chemical devices in 2D, 2D axisymmetric and 3D geometry, comparison of results | 2 |
| Pr18 | Simulation of a single-phase turbulent flow in various chemical devices in 2D, 2D axisymmetric and 3D geometry, application of different turbulence models, comparison of results | 2 |
| Pr19 | Simulation of the heat conduction in various chemical apparatuses | 2 |
| Pr10 | Simulation of the heat conduction with convection and radiation in various chemical apparatuses | 2 |
| Pr21 | Simulation of a flow with diffusion and chemical reaction | 2 |
| Pr22 | Simulation of a one phase isothermal, unsteady flow | |
| Pr23 | Simulation of a one phase transient flow with heat transfer | 2 |
| Pr24 | Simulation of a multiphase flow with the use of VOF model | 2 |
| Pr125 | Simulation of a gas-solid flow with the use of Euler-Euler model | 2 |
| Pr26 | Simulation of a liquid-liquid flow with the use of Euler-Euler model | 2 |
| Pr27 | Determination of particle trajectories in a multiphase flow using the Euler-Lagrange model | 2 |
| Pr28 | Project of the optimalization of a jet pump by means of CFD methods | 2 |
| Pr29 | Project of the optimalization of a heat exchanger by means of CFD methods | 2 |
| Pr30 | Test III | 2 |
| | Total hours | **60** |

| **TEACHING TOOLS USED** |
|---|
| N1. Lecture with multimedia presentation<br>N2. Computer simulation |

**EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT**

| **Evaluation** (F – forming during semester), P – concluding (at semester end) | Learning outcomes code | Way of evaluating learning outcomes achievement |
|---|---|---|
| P (lecture) | PEU_W01 | Final examination |
| F1 | PEU_U01<br>PEU_U02<br>PEU_U03 | Test I |
| F2 | PEU_U01<br>PEU_U02<br>PEU_U03 | Test II |
| F3 | PEU_U01 | Test III |
| F4 | PEU_U01<br>PEU_U02<br>PEU_U03<br><br>PEU_K01 | Evaluation of the project |

P = (F1 + F2 + F3+F4)/4 Each test and project must be passed with a positive grade.

3,0 if 3,00 ≤ P < 3,25

3,5 if 3,25 ≤ P < 3,75

4,0 if 3,75 ≤ P < 4,25

4,5 if 4,25 ≤ P < 4,75

5,0 if 4,75 ≤ P

## PRIMARY AND SECONDARY LITERATURE

**PRIMARY LITERATURE:**


[1] [1] J. D. Anderson, Computational Fluid Dynamics: The Basics with Application, McGraw-Hill, New York 1995

[2] [2] R. Shefflan, Teach Yourself the Basics of AspenPlus, John Wiley & Sons, 2011


**SECONDARY LITERATURE:**


[1] Ansys Fluent Help

[2] Comsol Multiphysics Help

[3] R. Smith, Chemical Process Design and Integration, Wiley 2005 R. Turton et al., Analysis, Synthesis, and Design of Chemical Processes, Prentice Hall 2009


**SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)**


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