POZNAN UNIVERSITY OF TECHNOLOGY

EUROPEAN CREDIT TRANSFER AND ACCUMULATION SYSTEM (ECTS)

COURSE DESCRIPTION CARD - SYLLABUS

Course name
Modeling and simulations [S2TCh2E-KiN>MiS]

Course

Field of study	Year/Semester
Chemical Technology	2/3
Area of study (specialization)	Profile of study
Composites and Nanomaterials	general academic
Level of study	Course offered in
second-cycle	english
Form of study	Requirements
full-time	compulsory

Number of hours

Lecture	Laboratory classes	Other (e.g. online)
15	0	0
Tutorials	Projects/seminars	
0	15	

Number of credit points

2,00

Coordinators

dr inż. Maciej Staszak
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Lecturers

Prerequisites

Student has knowledge of mathematics to the extent that allows him to use mathematical methods to describe chemical processes and make calculations needed in engineering practice. Student has knowledge in the basic field related to the selection of materials used in the construction of chemical equipment and installations. Student knows the basics of kinetics, thermodynamics and catalysis of chemical processes.

Course objective

The aim of this course is to present and learn issues related to modelling and simulation of chemical processes in flow systems, and learn how to model and design using CFD technique.

Course-related learning outcomes

Knowledge:
The student acquires knowledge in the field of model building and simulation calculations using the Computational Fluid Dynamics technique. The student knows how to build equations describing flow processes, including the Navier-Stokes equation, Fick's law, Maxwell-Stefan's law. The student understands the essence of building models, applying simplifying assumptions, using analogous models,

learning about the nature of processes by studying true, neutral and false models. (K_W01, K_W03, K_W06, K_W07)
The student acquires knowledge in the area of construction of two and three-dimensional spatial models of simple flow in pipeline, tank. The student is able to define the problem in the sense required by CAD tools. He also knows the importance of correct definition of the initial and boundary conditions and their impact on the constructed model. The student understands the necessity of using numerical procedures by the software and their significant influence on the way of calculation. (K_W01, K_W03, K_W06, K_W07)

Skills:
The student is able to formulate a description of processes in the sense of model mathematical equations. The student identifies the key elements of the description of the modelled process, which must be taken into account in building the model. The student is able to make decisions concerning the choice of flow models, diffusional mass transport, determination of initial and boundary conditions for the model being built. (K_U01, K_U06, K_U07, K_U14)
The student can work in a complex CAD environment. Using the Ansys platform, the student is able to select and use appropriate tools and connect them with selected design relationships. The student understands the order of selection of individual design steps. The student is able to analyze the results obtained in the zerodimensional sense and in the spatial distribution of results. (K_U01, K_U06, K_U07, K_U14)

Social competences:
The student is aware of the social impact of digital simulation tools. (K_K02)
The student is aware of the cost of the calculations. In addition, the student understands the impact of the applied digital tools on the functioning of society and wider knowledge of nature. (K_K02)

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Semester evaluation of the completed project, consisting of a preliminary pre-project analysis, the quality of the completed project and the preparation of the final report.

Programme content

Lecture: Model theory, models in science. Navier-Stokes flow equation for real fluids. Physical relationship for fluids, viscous stress strain tensor. Diffusion modelling in Fick's law, diffusion modelling in Maxwell-Stefan's law. Estimation of diffusion coefficients for gases, liquids, in infinitely small and current concentrations. Diffusion in multicomponent systems. Modelling the course of chemical, homo and heterogeneous reactions. Introduction to finite element technique.
Project: Modeling of single-component flow systems, multi-component flows, flows with chemical reactions and multiphase flows. Analysis of the results obtained using linear, planar and volumetric geometries. The integral representation of the results, transition from spatial distributions of the obtained variables to classical engineering description.

Teaching methods

Presentation at the lecture.
Project: Extensive presentation of the functions and operations of the design support tool - Ansys, Fluent, a tool for creating geometry and mesh. Detailed overview of the individual available functions. Detailed analysis and explanation of how to declare chemical reaction kinetics. Presentation of methods of including chemical catalysts. Based on the presented examples, students perform preliminary, test designs on simple spatial objects during the classes. At this stage, the teacher assists students in the use of the CAD tool.
During the realization of the target semester project, the students are assisted in the functioning of the Ansys platform, however, they make design decisions for which they are responsible. All solutions concerning definition of streams, use of models, selection of boundary conditions, numerical settings, constructional dimensions are the students' responsibility.

Bibliography

Basic:

Basics of Fluid Mechanics and Introduction to Computational Fluid Dynamics, Titus Petrila, Damian Trif, dostęp: https://link.springer.com/book/10.1007/b102528
Computational Methods for Fluid Dynamics, Joel H. Ferziger, Milovan Perić, Robert L. Street, dostęp: https://link.springer.com/book/10.1007/978-3-319-99693-6

Additional:
Computational Methods for Fluid Dynamics, Joel H. Ferziger, Milovan Perić, Robert L. Street, dostęp: https://link.springer.com/book/10.1007/978-3-319-99693-6
Chemical Reactor Modeling, Multiphase Reactive Flows, Hugo A. Jakobsen, Dostęp: https://link.springer.com/book/10.1007/978-3-319-05092-8

Breakdown of average student's workload

	Hours	ECTS
Total workload	50	2,00
Classes requiring direct contact with the teacher	30	1,00
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	20	1,00