GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Information technology tools in chemical technology and engineering, PG_00069293		
Field of study	Narzędzia informatyczne w technologii i inżynierii chemicznej		
Date of commencement of studies	February 2025	Academic year of realisation of subject	2025/2026
Education level	second-cycle studies	Subject group	
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	Polish
Semester of study	2	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Process Engineering and Chemical Technology -> Faculty of Chemistry -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Robert Aranowski	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	30.0	0.0	0.0	15.0	45

E-learning hours included: 0.0

Learning activity and number of study hours

Learning activity	Participation in didactic classes included in study plan	Participation in consultation hours	Self-study	SUM
Number of study hours	45	5.0	25.0	75

Subject objectives

The aim of the course is to present practical applications of digital tools in chemical engineering and to develop students ability to use intuitive computational environments. The course focuses on applying simulation methods and data analysis techniques to solve real engineering problems, with particular emphasis on a practical approach to information technologies commonly used in the chemical industry.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_U04] predicts the properties of the materials obtained and the course of processes involving them, based on knowledge of technology and related fields and computer methods of data analysis, modelling and simulation	Student potrafi skutecznie współpracować w zespole projektowym, przyjmując różne role i odpowiedzialności podczas realizacji zadań inżynierskich. EN: The student is capable of effective teamwork, assuming various roles and responsibilities in the implementation of engineering tasks.	[SU1] Ocena realizacji zadania
[K7_W03] selects methods of data analysis, including statistical and modelling, useful for solving scientific and technological problems	The student is able to select appropriate data analysis methods, including statistical and modeling techniques, to solve engineering and technological problems in chemical engineering.	[SW3] Ocena wiedzy zawartej w opracowaniu tekstowym i projektowym
[K7_U06] applies computer, statistical and specialised database methods to solve scientific and technological problems in technology and related fields	The student can apply computational tools, statistical methods, and specialized databases for the analysis, modeling, and simulation of chemical processes.	[SU1] Ocena realizacji zadania
[K7_K03] can interact and work in a group, taking on a variety of roles	The student is capable of effective teamwork, assuming various roles and responsibilities in the implementation of engineering tasks.	[SK2] Ocena postępów pracy

Subject contents

Course content – exercises

1. Wprowadzenie do narzędzi informatycznych w inżynierii chemicznej
2. Bilans masowy i energetyczny podejście numeryczne
3. Wprowadzenie do modelowania matematycznego procesów
4. Modelowanie wymiany ciepła teoria i przykłady
5. Kolumny absorpcyjne i destylacyjne
6. Metody numeryczne i aproksymacja danych pomiarowych
7. Optymalizacja procesów technologicznych
8. Symulatory procesowe open-source i komercyjne
9. Przegląd dostępnych symulatorów i ich zastosowań
10. Wizualizacja wyników i raportowanie
11. Przygotowanie problemu inżynierskiego do rozwiązania w grupie 3-4 osobowej
12. Prezentacje zespołowe, ocena równorzędna.

Course content – seminar

1. Introduction to computer tools in chemical engineering.
2. Mass and energy balance numerical approach.
3. Introduction to mathematical modeling of processes.
4. Heat transfer modeling theory and examples.
5. Absorption and distillation columns.
6. Numerical methods and approximation of experimental data.
7. Optimization of technological processes.
8. Open-source and commercial process simulators.
9. Overview of available simulators and their applications.
10. Visualization of results and reporting.
11. Preparation of an engineering problem to be solved in teams of 34 students.
12. Team presentations and peer evaluation.

Prerequisites and co-requisites

Knowledge of the basics of chemical technology, chemical engineering, and computer skills.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Seminar: Based on a Kahoot quiz.	60.0%	50.0%
Exercises: Based on peer assessment of group presentation	60.0%	50.0%

Recommended reading

Basic literature

1. Pakowski Zdzisław, Symulacja procesów inżynierii chemicznej: teoria i zadania rozwiązane programem Mathcad, Wydaw. Politech. Łódzkiej, Łódz, 2001.
2. H.S. Fogler, Elements of Chemical Reaction Engineering, Fourth Ed., Prentice Hall PTR, New Jersey, 2005.
3. Beers K.J., Numerical Methods for Chemical Engineering. Applications in MATLAB®, Cambridge University Press, New York, 2007
4. Walas S. M. Chemical Process Equipment: Selection and Design Butterworth-Heinemann, 2013.
5. Fogler H. S. Elements of Chemical Reaction Engineering Prentice Hall, 2020. (Podstawowa pozycja do reakcji i modelowania kinetycznego)
6. Sanders R. E. Chemical Process Safety Butterworth-Heinemann, 2015.

Supplementary literature

1. Bockhorn H. (Ed.) Mathematical Modeling of Chemical Engineering Processes, Elsevier, 1998.
2. D. Himmelblau Basic Principles and Calculations in Chemical Engineering, Prentice Hall, 8th ed., 2012.
3. Luyben W. L. Process Modeling, Simulation and Control for Chemical Engineers McGraw-Hill, 1990.
4. Smith R. Chemical Process: Design and Integration Wiley, 2016.
5. Perkins J. D., Pistikopoulos E. N. Process Systems Engineering Elsevier, 2007.
6. Stephanopoulos G. Chemical Process Control: An Introduction to Theory and Practice Prentice Hall, 1984.
7. Bequette B. W. Process Dynamics: Modeling, Analysis and Simulation Prentice Hall, 1998.

eResources addresses

Supplementary

https://esupport.aspentech.com/ - Training “Aspen Plus for Beginners” available after registration.

https://www.youtube.com/results?search_query=ChemCAD+simulation+tutorial - Free ChemCAD tutorials

https://www.scilab.org/tutorials - Free Scilab tutorials

Example issues/ example questions/ tasks being completed

Prepare a Scilab/Matlab script to calculate the flame temperature for the complete combustion in air of a gaseous hydrocarbon with the formula CH. The process involves partial thermal dissociation of CO and HO. Assume that the dissociation reactions reach equilibrium at the temperature at which the process occurs. The fuel and air are introduced at room temperature (25°C) and atmospheric pressure, and the oxygen-to-fuel ratio corresponds to the stoichiometric ratio. Test the script for the following hydrocarbons: ethane, ethylene, propane, propene, acetylene, n-butane, 2-methylpropane, and 1,2-butadiene.

Practical activites within the subject

Not applicable

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