GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Computer-Aided Design, PG_00060870		
Field of study	Chemical Technology		
Date of commencement of studies	October 2025	Academic year of realisation of subject	2027/2028
Education level	first-cycle studies	Subject group	Obligatory subject group in the field of study
Mode of study	Full-time studies	Mode of delivery	at the university
Year of study	3	Language of instruction	Polish
Semester of study	5	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Department of Process Engineering and Chemical Technology -> Faculty of Chemistry -> Faculties of Gdańsk University of Technology		
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	15.0	0.0	0.0	30.0	0.0	45
E-learning hours included: 0.0						
eNauczanie source address: https://enauczanie.pg.edu.pl/2025/course/view.php?id=2916						

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	3.0	27.0	75

Subject objectives

The aim of the course is to familiarize students with the latest software used in the design of technological processes, including software for making engineering drawings, technological calculations and process simulations.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K6_U08] Is able to select elements of automatic control systems for simple technological processes and use computer programs to control and optimize chemical processes.	Student is able to build a simplified mathematical model of a technological process (e.g. reactor, heat exchanger, absorption column) for the purpose of dynamic and regulatory analysis.	[SU1] Assessment of task fulfilment
[K6_W05] Has knowledge of electrical engineering, automation and computer science, including the operation of measurement and control systems	Student has knowledge of mathematical modeling of regulators and representation of technological processes in the form of dynamic models used in control systems.	[SW3] Assessment of knowledge contained in written work and projects

Subject contents	Course content – lecture **Lecture Contents** 1. Organizational information. Introduction to Computer-Aided Design. 2. Concepts of empirical, analog, physical, and mathematical models; presentation of real problems of design, modeling, and optimization. 3. Simulation models. Principles of process simulation: systems with lumped and distributed parameters in steady and unsteady states. 4. Introduction to solving simulation and design problems. Mathematical description of chemical process operations, balance equations for model units. 5. Example of material and energy balancing for technological processes in the steady state. 6. Example of material and energy balancing for technological processes in the unsteady state. 7. Calculation of equilibrium constants: empirical models (ESSO, ideal solutions, Henrys constant), SoaveRedlichKwong (SRK) model, GraysonStreed model, modified ChaoSeader model (GMAC). 8. Equations of state for real gases: limitations of the ideal gas model, virial equation of real gases, cubic models PengRobinson, BenedictWebbRubinStarling (BWRS), API SoaveRedlichKwong model. 9. Equations of state for real gases (continued): modified SoaveRedlichKwong (MSRK) model, extended SoaveRedlichKwong (TSRK) model, predictive SoaveRedlichKwong (PSRK) model, SAFT equation, ElliottSureshDonohue (ESD) model. 10. Modeling of phase equilibrium and chemical reactions using real-gas equation of state models. 11. Activity coefficient models: Van Laar, NRTL, Margules; activity coefficient models: GMAC (ChienNull), ScatchardHildebrand, Pitzer, MNRTL. 12. Group-contribution methods for determining activity coefficients: UNIQUAC and UNIFAC methods. 13. Computational examples of applying group-contribution methods to vaporliquid equilibrium calculations. 14. Thermodynamic properties estimated based on real-gas models: SoaveRedlichKwong, PengRobinson, RedlichKwong. 15. Test.
	Course content – project Project class contents: 1. Introduction to Scilab software. 2. Material balance of unit operations without chemical reaction. Example: a separation process. 3. Material balance of unit operations with chemical reaction. Calculations based on reaction kinetics and chemical equilibrium. 4. Heat balance of unit operations. Heat balance for isothermal and adiabatic operation. 5. The coupled mass-and-energy balance problem. 6. Calculations for unsteady (dynamic) processes. 7. Calculations for process systems with recycle. Example using the equation-oriented method; example using the sequential-modular method. 8. Calculations of gasliquid phase equilibria. 9. Parameter identification and data regression: fitting VLE/kinetic parameters in Scilab (nonlinear regression). 10. ChemCAD introduction. Building a model (flowsheet, stream definitions, selection of thermodynamic model). 11. Simulation of a distillation column in design and simulation modes. Reactive distillation. 12. Process flows with chemical reaction. Types of reactors.

	13. Heat exchange and energy-use optimization. 14. Recycle issues in ChemCAD. 15. Assessment: case study using ChemCAD and Scilab.
Prerequisites and co-requisites	Computer skills, knowledge of the Office suite and chemical unit processes.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
3 short Scilab/ChemCAD tests	60.0%	25.0%
Activity (mini quizzes)	60.0%	5.0%
Design challenge + presentation of results in groups of 3-4 people	60.0%	55.0%
Conceptual Colloquium - Lecture	60.0%	15.0%

Recommended reading

Basic literature	1. H.S. Fogler, Elements of Chemical Reaction Engineering, Fourth Ed., Prentice Hall PTR, New Jersey, 2005. 2. Beers K.J., Numerical Methods for Chemical Engineering. Applications in MATLAB®, Cambridge University Press, New York, 2007 3. Walas S. M. Chemical Process Equipment: Selection and Design Butterworth-Heinemann, 2013. 4. Fogler H. S. Elements of Chemical Reaction Engineering Prentice Hall, 2020. (Podstawowa pozycja do reakcji i modelowania kinetycznego) 5. Sanders R. E. Chemical Process Safety Butterworth-Heinemann, 2015.
Supplementary literature	1. Heermann Dieter W., Podstawy symulacji komputerowych w fizyce, Warszawa, Wydaw. Nauk.-Tech, 1997. 2. Jach Karol, Komputerowe modelowanie dynamicznych oddziaływań ciał metodą punktów swobodnych, praca zbiorowa, Warszawa, Wydaw. Naukowe PWN, 2001. 3. Winkowski Józef, Programowanie symulacji procesów, Warszawa, Wydaw. Nauk.-Tech., 1974. 4. James A., Modelowanie matematyczne w oczyszczaniu ścieków i ochronie wód, Arkady, Warszawa 1986.
eResources addresses	

Example issues/ example questions/ tasks being completed	Prepare a Scilab script that calculates the flame temperature for complete combustion of a gaseous hydrocarbon with the formula C_KH_L in air. The process involves partial thermal dissociation of CO_2 and H_2O. Assume that the dissociation reactions reach equilibrium at the reaction temperature. Assume that the fuel and air are introduced at room temperature (25°C) and atmospheric pressure, and that the oxygen/fuel ratio corresponds to the stoichiometric ratio. Verify the script's operation for the following hydrocarbons: ethane, ethylene, propane, propene, acetylene, n-butane, 2-methylpropoate, and 1,2-butadiene.
Practical activites within the subject	Not applicable