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 2023	Academic year of realisation of subject	2025/2026
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 -> Wydziały Politechniki Gdańskiej		
Name and surname of lecturer (lecturers)	Subject supervisor	dr inż. Robert Aranowski	
	Teachers	dr inż. Robert Aranowski	

Lesson types and methods of instruction

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=1070

Moodle ID: 1070 Komputerowe Wspomaganie Projektowania, Technologia Chemiczna, 2025/26-1 https://enauczanie.pg.edu.pl/2025/course/view.php?id=1070

Additional information:
Link to supplementary materials in the e-learning system:

https://enauczanie.pg.edu.pl/2025/course/view.php?id=1070

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	<table><tr><th>Course outcome</th><th>Subject outcome</th><th>Method of verification</th></tr><tr><td>[K6_U04] performs basic design calculations of selected processes and unit operations, is able to calculate and select the basic apparatus of chemical industry in a process line</td><td>Balances and input data – can formulate assumptions, select a thermodynamic model and perform mass and energy balances for simple systems (in steady and transient states), obtaining a complete flux table.</td><td>[SU1] Assessment of task fulfilment</td></tr><tr><td>[K6_W06] has knowledge of information technology and computer-aided design, the use of databases in technological design</td><td>The student has knowledge of data flow in CAD programs (ChemCAD/Scilab) and the use of databases: sets of components, thermophysical properties, model parameters (EOS, NRTL/ UNIQUAC/UNIFAC), kinetics and costs.</td><td>[SW3] Assessment of knowledge contained in written work and projects</td></tr><tr><td>[K6_U10] is able to select elements of automatic control systems for simple technological processes. Is able to use computer programmes supporting the implementation of tasks typical of control and optimisation of chemical processes</td><td>Efficiently uses Scilab for modeling and control, as well as a process simulator (ChemCAD) to obtain operating points/ parameters, and documents the results with scripts and reports.</td><td>[SU1] Assessment of task fulfilment</td></tr></table>
Subject contents	Lecture contents: 1. Organizational information. Introduction to Computer-Aided Design (CAD). CAD-type software tools and their practical relevance across engineering fields. 2. Concepts of empirical, analog, physical, and mathematical models; presentation of real-world problems in design, modeling, optimization, and process scale-up. 3. Simulation models: black-box and deterministic models; software for process simulation and design. Principles of process simulation: lumped-parameter vs. distributed-parameter systems in steady-state and dynamic (unsteady) operation. 4. Introduction to solving simulation and design problems. Mathematical description of chemical process operations; types of mathematical models; balance equations for model unit operations; mass and energy balance equations. 5. Example: material and energy balancing of technological processes in steady state. 6. Example: material and energy balancing of technological processes in unsteady (dynamic) state. 7. Calculation of equilibrium constants: empirical models (e.g., ESSO, ideal solutions, Henrys law), SoaveRedlichKwong (SRK) model, GraysonStreed model, modified ChaoSeader (GMAC) model. 8. Equations of state for real gases: limitations of the ideal-gas model; the virial equation for real gases; cubic EOS: PengRobinson, BenedictWebbRubinStarling (BWRS), API SoaveRedlichKwong. 9. Equations of state for real gases (continued): Modified SRK (MSRK), Extended/Two-parameter SRK (TSRK), Predictive SRK (PSRK), SAFT equation, ElliottSureshDonohue (ESD) model. 10. Modeling of phase equilibria and chemical reactions using real-gas EOS models. 11. Activity-coefficient models: van Laar, NRTL, Margules; activity-coefficient models (continued): GMAC (ChienNull), ScatchardHildebrand, Pitzer, mNRTL. 12. Group-contribution methods for activity coefficients: UNIQUAC and UNIFAC. 13. Computational examples using group-contribution methods to determine vaporliquid equilibrium (VLE). 14. Thermodynamic properties estimated from real-gas models: SoaveRedlichKwong, PengRobinson, RedlichKwong. 15. Test 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
Conceptual Colloquium - Lecture	60.0%	15.0%
Activity (mini quizzes)	60.0%	5.0%
3 short Scilab/ChemCAD tests	60.0%	25.0%
Design challenge + presentation of results in groups of 3-4 people	60.0%	55.0%

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	Basic https://www.scilab.org/tutorials - Scilab Tutorials https://www.youtube.com/results?search_query=ChemCAD+simulation+tutorial - ChemCAD tutorial videos on Youtube

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.
Work placement	Not applicable