



Subject card

Subject name and code	Computer-Aided Design, PG_00060870						
Field of study	Chemical Technology						
Date of commencement of studies	October 2026		Academic year of realisation of subject		2028/2029		
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						
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.		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		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 Introduction to computer-aided design. Concepts of empirical, analogue, physical and mathematical models. Examples of real-world design, modelling and optimization problems. Simulation models. Principles of process simulation: lumped- and distributed-parameter systems under steady-state and dynamic conditions. Introduction to solving simulation and design problems. Mathematical description of chemical processes and balance equations for model process units. Material and energy balancing of technological processes under steady-state and dynamic conditions. Calculation of equilibrium constants: empirical models (ESSO, ideal solutions, Henry's law), Soave–Redlich–Kwong (SRK), Grayson–Streed and modified Chao–Seader (GMAC) models. Equations of state for real gases: limitations of the ideal gas model, virial equation, Peng–Robinson and Soave–Redlich–Kwong cubic equations of state, and BWRS, API-SRK, MSRK, TSK, PSRK, SAFT and Elliott–Suresh–Donohue (ESD) models. Modelling of phase and chemical reaction equilibria using real-gas models. Activity coefficient models: van Laar, NRTL, Margules, Chien–Null (GMAC), Scatchard–Hildebrand, Pitzer and MNRTL. UNIQUAC model and UNIFAC group contribution method. Examples of using models to determine vapour–liquid equilibrium. Determination of thermodynamic properties using the Redlich–Kwong, Soave–Redlich–Kwong and Peng–Robinson equations of state.		
	Course content – project Introduction to a numerical computing environment and its application to engineering calculations. Material balancing of process units without chemical reactions using separation processes as examples, and of units involving chemical reactions, including reaction kinetics and chemical equilibrium. Energy balancing of process units operating under isothermal and adiabatic conditions and simultaneous solution of mass and energy balances. Dynamic process calculations. Calculation of process systems with recycle streams using equation-oriented and sequential-modular approaches. Vapour–liquid equilibrium calculations. Parameter identification and data regression, including fitting of vapour–liquid equilibrium (VLE) and reaction kinetic model parameters using nonlinear regression in a numerical computing environment. Introduction to process simulation software. Development of process models: preparation of process flow diagrams, definition of streams and selection of thermodynamic models. Simulation of distillation columns in design and simulation modes and reactive distillation. Modelling of technological processes involving chemical reactions and selection of reactor models. Heat transfer modelling and optimization of energy consumption. Calculation of process systems with recycle streams using a process simulator. A case study integrating a numerical computing environment and process simulation software for technological process modelling and simulation.		
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	Supplementary https://help.scilab.org/?utm_source=chatgpt.com - Official documentation of the Scilab numerical computing environment. It provides descriptions of functions, computational methods and tools useful for solving equations, data analysis, regression, optimization, and process modelling and simulation. https://webbook.nist.gov/chemistry/?utm_source=chatgpt.com - An online database of the National Institute of Standards and Technology providing evaluated physicochemical and thermodynamic data. It includes thermochemical data, phase-change properties, equilibrium data and fluid properties useful in process modelling and simulation. https://www.chemstations.com/?utm_source=chatgpt.com - Official website of the CHEMCAD process simulator. It provides information on process modelling and simulation, available computational modules and supporting resources for the application of CHEMCAD in chemical process design.
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 ($25^\circ C$) 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-methylpropene, and 1,2-butadiene.	
Practical activities within the subject	Not applicable	

Document generated electronically. Does not require a seal or signature.