



## Subject card

Subject name and code	Methodology of simulation and optimization of technological processes , PG_00035159						
Field of study	Engineering and Technologies of Energy Carriers						
Date of commencement of studies	February 2023	Academic year of realisation of subject			2023/2024		
Education level	second-cycle studies	Subject group			Optional subject group Subject group related to practical vocational preparation		
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	practical profile	Assessment form			assessment		
Conducting unit	Department of Process Engineering and Chemical Technology -> Faculty of Chemistry						
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	30.0	0.0	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 present (theoretically and practically) modern simulation tools and solving process problems.						
Learning outcomes	Course outcome	Subject outcome			Method of verification		
	K7_U05	Student is able to use teamwork skills when formulating models of technological processes			[SU1] Assessment of task fulfilment		
	K7_U06	Student is able to use the costing estimating module during process simulations using PetroSIM software			[SU4] Assessment of ability to use methods and tools		
	K7_W10	Student is able to choose the appropriate mathematical model of calculations of chemical equilibrium and thermal effects of the process			[SW3] Assessment of knowledge contained in written work and projects		
	K7_W13	Student is able to choose the right mathematical model to simulate the work of industrial devices and apparatus			[SW3] Assessment of knowledge contained in written work and projects		
K7_W04	Student is able to simulate an industrial processes using PetroSIM software			[SW3] Assessment of knowledge contained in written work and projects			
Subject contents	Concepts of empirical, analog, physical and mathematical model; Introduction to the real problems of design, modeling, optimization and scaling up of processes. Estimation of measuring errors and calculation of additive errors, factor design and curtailed sampling plans for modeling of physical and chemical processes. Utilization of statistical methods to control industrial processes. Mathematical description of chemical processes, types of mathematical models, the balance equations for apparatus models, the equations of mass and energy balances. Simulation models: black box models, deterministic models, software for simulation and design processes. Processes simulation rules: objects with lumped and distributed parameters in a steady and transient state. Approximation and prediction properties of the substance: density, viscosity, the critical parameters, the liquid proper volume, gas proper volume, volatility of gases and liquids, phase equilibrium (equation of Margules van Laar and Wilson). Chemical equilibrium, calculating the concentrations at steady state. A database of physicochemical properties of pure substances, properties of mixtures and phase equilibrium. Modern simulation methods, solving process problems, simulation of mass flows, full simulation and optimization of steady-state processes. Simulation of chemical processes using the ChemCAD software in steady state and dynamic mode.						

Prerequisites and co-requisites	Knowledge of unit processes, including the distillation and rectification, mass and energy transfer. Knowledge of the basic equipment and apparatuses used in the chemical industry. Knowledge about basic physico-chemical parameters of matter.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Project	60.0%	50.0%
	Test	60.0%	50.0%
Recommended reading	Basic literature	<ol style="list-style-type: none"> <li>1. Leigh J. R., Modelling and simulation, London, Peter Peregrinus, 1983.</li> <li>2. William Luyben, Process Modeling, Simulation and Control for Chemical Engineers, McGraw-Hill Chemical Engineering Series, 1996.</li> </ol>	
	Supplementary literature	<ol style="list-style-type: none"> <li>1. Octave Levenspiel, Chemical reaction Engineering, John Wiley &amp; Sons, 1999.</li> </ol>	
	eResources addresses	Adresy na platformie eNauczenie: Metodologia symulacji i optymalizacji procesów technologicznych, wykład, liTNE, 2023-24, semestr zimowy - Moodle ID: 32003 <a href="https://enauczenie.pg.edu.pl/moodle/course/view.php?id=32003">https://enauczenie.pg.edu.pl/moodle/course/view.php?id=32003</a>	
Example issues/ example questions/ tasks being completed	<p>In the production of ethyl propionate, 60% ethyl alcohol is mixed with 40% propionic acid. The reaction is carried out with simultaneous removal of the products in a distillation column. The inlet acid temperature is 30C and the pressure was 1 atm. The inlet temperature of the alcohol is 40C and the pressure 2 atm. The distillation column operates at atmospheric pressure and is equipped with 20 trays. The efficiency of the highest and lowest trays is 0.8 and 0.7, respectively. The acid stream is fed to the 7th tray and the alcohol stream to the 9th tray. The column does not have a condenser. The reflux ratio is 0.8 and the boiler power is 2 MW. As a column simulation model, use the "Equilibrium model". The volume of the liquid on the trays is 5 dm<sup>3</sup>. The values of the coefficients for the change of the reaction equilibrium constant with temperature are as follows: A = 10.82; B=28.96; C=0.5385; D=0.00016. The overhead product of the first column should be separated in the second distillation column in which no chemical reaction takes place. Use the "Equilibrium model" as a simulation model for the operation of the 2nd column which has 20 theoretical trays. By changing the reflux coefficient and boiler power, optimise ethyl propionate production efficiency with a purity of at least 80%. Generate a material and energy balance of the process and a column profile graph using the ChemCAD simulator.</p>		
Work placement	Not applicable		