Zachodniopomorski Uniwersytet Technologiczny w Szczecinie

Faculty of Chemical Technology and Engineering

Field of study	Chemical Engineering		
Mode of study	stationary	*Level*	first cycle
Graduate's qualification	inżynier		
Area(s) of study	nauki techniczne		
Educational profile	general academic		
Module			
Course unit	**Introduction to Modeling, Simulation and Numerical Methods Applied to Chemical Engineering**		
Code	ChEn_1A_S_C08a		
Field of specialisation			
Administering faculty	Institute of Chemical Engineering and Environmental Protection Processes		
ECTS	5,0	*ECTS (forms)*	5,0
Form of course credit	credits	*Language*	english
Electives	3	*Elective group*	

Form of instruction	*Code*	*Semester*	*Hours*	*ECTS*	*Weight*	*Credit*
lecture	W	4	30	2,0	0,50	credits
laboratory course	L	4	45	3,0	0,50	credits

Leading teacher	Pianko-Oprych Paulina (Paulina.Pianko@zut.edu.pl)
Other teachers	Aleksandrzak Tomasz (Tomasz.Aleksandrzak@zut.edu.pl), Ambrożek Bogdan (Bogdan.Ambrozek@zut.edu.pl), Pianko-Oprych Paulina (Paulina.Pianko@zut.edu.pl), Story Anna (Anna.Story@zut.edu.pl), Witkiewicz Konrad (Konrad.Witkiewicz@zut.edu.pl), Ziętarska Katarzyna (kzietarska@zut.edu.pl)

Prerequisites	
W-1	Mathematics
W-2	Physics
W-3	Thermodynamics

Module/course unit objectives	
C-1	This course focuses on the use of modern computational and mathematical techniques in chemical engineering. Starting from a discussion of linear systems as the basic computational unit in scientific computing, methods for solving sets of nonlinear algebraic equations, ordinary differential equations, and differential-algebraic (DAE) systems are presented. Mathematical modelling of steady-state and dynamic chemical engineering systems is discussed. Basic optimization theory and algorithms with applications to chemical engineering problems are discussed. Process simulation techniques are presented. Utilization of mass, energy and momentum balances and rate processes to describe the behaviour of chemical engineering systems will be shown. The use of these techniques will be demonstrated throughout the course in the MATLAB and Aspen TECH computing environments.

Course content divided into various forms of instruction		*Number of hours*
T-W-1	Formulation of physicochemical problems (AT, AB, WK)	3
T-W-2	Classification of mathematical models (AT, AB, WK)	3
T-W-3	Reducing mathematical models (AT, AB, WK)	3
T-W-4	Error estimations (AT, AB, WK)	3
T-W-5	Numerical methods for ordinary differential equations, ODEs (AT, AB, PPO, SA, WK)	6
T-W-6	Methods for boundary value problems (AT, AB, PPO, SA, WK)	3
T-W-7	Numerical methods for partial differential equations, PDEs (AT, AB, PPO, SA, WK)	3
T-W-8	Statistical analysis of mathematical models (AT, AB, PPO, SA, WK)	6
T-L-1	MATLAB Basics (AT, AB, WK, ZK)	3
T-L-2	Curve-Fitting (AT, AB, WK, ZK)	3
T-L-3	Numerical Integration (AT, AB, WK, ZK)	3
T-L-4	A System of Algebraic Equations (AT, AB, WK, ZK)	3
T-L-5	Solving Differential Equations (AT, AB, PPO, SA, WK, ZK)	6
T-L-6	Solving selected problems from chemical engineering in Matlab (AT, AB, PPO, SA, WK, ZK)	9
T-L-7	Introducing Aspen Plus (PPO, SA)	3
T-L-8	Aspen Plus Flowsheet Features (PPO, SA)	6
T-L-9	Simulation of selected problems from chemical engineering in Aspen Plus (PPO, SA)	9

Student workload - forms of activity		*Number of hours*
A-W-1	Lecture participation	30
A-W-2	Individual literature studies	20
A-W-3	One-on-one teaching consultations	5
A-W-4	Repetition of the lecture content to the written test	5
A-L-1	Classroom participation	45
A-L-2	Preparation of reports in MATLAB	20
A-L-3	Preparation of reports in Aspen Plus	10
A-L-4	One-on-one teaching consultations	6
A-L-5	Literature studies	10

Teaching methods / tools	
M-1	Preparation of a multimedia for of lecture presentation
M-2	Numerical analysis by solving chemical engineering problems using MATLAB.
M-3	Numerical analysis by solving chemical engineering problems using Aspen TECH.

Evaluation methods (F - progressive, P - final)		
S-1	P	Written final exam based on the lecture contents.
S-2	F	Mid-term exam 1 - MATLAB.
S-3	F	Mid-term exam 2 - Aspen TECH

Designed learning outcomes	Reference to the learning outcomes designed for the fields of study	Reference to the learning outcomes defined for the particular areas of education	Reference to learning outcomes leading to the degree of "inżynier"	Course objectives	Course content	Teaching methods	Evaluation methods
Knowledge							
ChEn_1A_C08a_W01 Students can formulate mathematical models and translate them into forms appropriate for computation. Students can identify problem structure, scale and complexity.	ChEn_1A_W06 ChEn_1A_W07 ChEn_1A_W08 ChEn_1A_W15	P6S_WG_TA11	P6S_WG_IA11	C-1	T-W-1 T-W-5 T-W-2 T-W-6 T-W-3 T-W-7 T-W-4 T-W-8	M-1	S-1
Skills							
ChEn_1A_C08a_U01 Students have a working knowledge of MATLAB and AspenTech. Students can produce working code to solve com- mon chemical engineering problems including steady-state and dynamic simulatin. Students can readily interpret results and output.	ChEn_1A_U01 ChEn_1A_U03 ChEn_1A_U05 ChEn_1A_U07 ChEn_1A_U08 ChEn_1A_U09 ChEn_1A_U16	P6S_UO P6S_UU P6S_UW_TA11 P6S_UW_TA12 P6S_UW_TA14	P6S_UW_IA11 P6S_UW_IA12 P6S_UW_IA14	C-1	T-L-1 T-L-6 T-L-2 T-L-7 T-L-3 T-L-8 T-L-4 T-L-9 T-L-5	M-2 M-3	S-2 S-3
Other social / personal competences							
ChEn_1A_C08a_K01 Students can select methods and software based on problem types. Students can defend the selection of methods and software based on characteristics such as convergence properties, time complexity, storage complexity, accuracy, and limitations with respect to specific problems.	ChEn_1A_K01 ChEn_1A_K03 ChEn_1A_K04 ChEn_1A_K05	P6S_KK P6S_KO P6S_KR		C-1	T-L-1 T-L-6 T-L-2 T-L-7 T-L-3 T-L-8 T-L-4 T-L-9 T-L-5	M-2 M-3	S-2 S-3

Required reading

1. R.G. Rice, D.D. Do, Applied mathematics and modeling for chemical engineers, John Wiley & Sons, Inc., New York, 2012

2. B.A. Finlayson, Introduction to chemical engineering computing, John Wiley & Sons, Inc., New Jersey, 2006

3. K.I.M. Al-Malah, MATLAB Numerical Methods with Chemical Engineering Applications, McGraw-Hill Education, 2014

4. K.I.M. Al-Malah, Aspen Plus Chemical Engineering Applications, John Wiley & Sons, Inc., New Jersey, 2017

Supplementary reading

1. Drfman K. D., Prodromos D., Numerical Methods with Chemical Engineer- ing Applications, Cambridge University Press,, 2017, 9781107135116