FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in Polish: Modelowanie procesów technologicznych
Name of subject in English: Process modeling in chemical technology
Main field of study: Chemical technology
Specialization: Technology of fine chemicals
Profile: academic
Level and form of studies: 2nd level, full-time
Kind of subject: obligatory
Subject code: TCC024007
Group of courses: NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	15		30		
Number of hours of total student workload (CNPS)	30		60		
Form of crediting	crediting with grade		crediting with grade		
For group of courses mark (X) final course					
Number of ECTS points	1		2		
including number of ECTS points for practical (P) classes			2		
including number of ECTS points for direct teacher-student contact (BK) classes	0.5		1		

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of physical chemistry: kinetics of complex chemical reactions, chemical equilibrium, thermodynamic functions.
2. Basic knowledge of differential and integral calculus.

SUBJECT OBJECTIVES

C1. To familiarize students with mathematical models of complex chemical processes.
C2. To familiarize students with the goals of modeling: simulation, optimization and controlling.
C3. Learning how to formulate and solve easy optimization problems.

SUBJECT LEARNING OUTCOMES

relating to knowledge:
The person who passed course:
PEK_W01 has a basic knowledge about models of chemical reaction processes,
PEK_W02 knows examples of application of modeling in process simulation and optimization
PEK_W03 has a basic knowledge about regressions analysis and optimization methods

relating to skills:
PEK_U01 is able to apply regression analysis in modeling of chemical reactions
PEK_U02 is able to numerically simulate the operation of a selected chemical reactor
PEK_U03 is able to optimize operating conditions of a selected chemical reactor

PROGRAMME CONTENT

Lectures		Number of hours
Lec1	Process modeling: physical object-mathematical model;	2

	illustrations with examples of processes running in chemical reactors.	
Lec2	Application of modeling. Simulation, optimization, control. The structure of the task: the process equations, boundary conditions, a steady state, the criterion (optimization),examples of solving methods.	2
Lec3	Process simulation: plug flow reactor (PFR) with reversible and exothermic reaction. Calculation of concentration and conversion under adiabatic or isothermal condition.	2
Lec4	Optimizing production costs: processes with without recycling of unreacted raw materials.	2
Lec5	Process optimization: optimum temperature profile, reversible and exothermic reaction, plug flow reactor, method of the calculus of variations.	2
Lec6	Process optimization: selection of optimum temperature and optimum conversion for reversible and exothermic reaction in series of CSTR.	2
Lec7	Example of process control with the feedback controller for three CSTR in series.	2
Lec8	Written credit.	1
	Total hours	**15**

Laboratory		**Number of hours**
Lab1 – Lab2	Regression analysis in modeling of chemical reactions kinetics; reaction order and reaction rate.	4
Lab3 – Lab4	Basics of PFR, CSTR and BATCH simulation. Gas phase reaction with variable volume at constant pressure (PFR) and with the constant volume and variable of pressure (BATCH), influence of a presence of an inert substance on the reaction yield.	4
Lab5 – Lab6	CSTR and PFR comparison. Simulation of CSTR in series: different types of complex reactions.	4
Lab7 – Lab8	Procedures for numerical integration (rectangular, trapezoidal and Simpson methods) and numerical differentiation supported by experimental data (CSTR, PFR).	4
Lab9	Determination of the optimal temperature profile for different types of reaction carried out in plug flow reactor (PFR).	2
Lab10	Determination of the optimal temperature profile for different types of reaction carried out in a single CSTR and in a sequence of CSTRs.	2
Lab11	Simulation of an adiabatic PFR: gas phase reaction, impact of inerts, $\Delta H(T)$ and $Cp(T)$ dependence.	2
Lab12 – Lab13	Simulation of selected reactor types under isothermal, adiabatic and non-adiabatic conditions.	4
Lab14	Written credit I.	2
Lab15	Written credit II.	2
	Total hours	**30**

TEACHING TOOLS USED

N1.Lecture with a multimedia presentation.
N2.Using the Excel + Solver software.
N3.Using the Polymath software.

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming (during semester), P – concluding (at semester end)	Learning outcomes number	Way of evaluating learning outcomes achievement
P (lecture)	PEK_W01 – PEK_W03	Written credit
F (laboratory)	PEK_U01 – PEK_U03	Written credit

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:
[1] W. Luyben, Chemical reactor design and control , Hoboken : Wiley-Interscience, 2007
[2] H. S. Fogler, Elements of Chemical Reaction Engineering Fourth Edition, Prentice Hall 2005

SECONDARY LITERATURE:
[1] J. M. Coulson, J. F. Richardson, Chemical Engineering, Pergamon Press, Oxford 1971
[2] R. E. Hayes Introduction to chemical reactor analysis CRC Press/Taylor & Francis, 2013.

SUBJECT SUPERVISOR (NAME AND SURNAME, E-MAIL ADDRESS)

dr. Bartłomiej M. Szyja (b.m.szyja@pwr.edu.pl) lecture
prof. dr hab. inż. Józef Hoffmann (jozef.hoffmann@pwr.edu.pl) laboratory