Zał. nr 5 do ZW 78/2023

Attachment no. 4. to the Program of Studies

FACULTY OF CHEMISTRY

SUBJECT CARD

Name of subject in Polish: Podstawy projektowania w technologii chemicznej
Name of subject in English: Fundamentals of chemical technology design
Main field of study (if applicable): all Faculty of Chemistry
Specialization (if applicable):
Profile: academic
Level and form of studies: 2nd level – supplementary semester, full-time
Kind of subject: obligatory
Subject code: W03W03-SM2030W, W03W03-SM2030P
Group of courses: NO

	Lecture	Classes	Laboratory	Project	Seminar
Number of hours of organized classes in University (ZZU)	30			30	
Number of hours of total student workload (CNPS)	75			50	
Form of crediting	crediting with grade, exam (2nd level in english)			crediting with grade	
For group of courses mark (X) final course					
Number of ECTS points	3			2	
including number of ECTS points for practical (P) classes				2	
including number of ECTS points for direct teacher-student contact (BU) classes	1,3			1,5	

PREREQUISITES RELATING TO KNOWLEDGE, SKILLS AND OTHER COMPETENCES

1. Knowledge of general chemistry: properties of substances, stoichiometry
2. Knowledge of physical chemistry: thermodynamics, kinetics
3. Knowledge of mathematics: differentiation, integration, differential equations

SUBJECT OBJECTIVES

C1 To familiarize with basic concepts and laws in the field of chemical technology
C2 To familiarize with material and thermal balances of the process.
C3 To familiarize with physicochemical properties of substances and methods of their evaluation
C4 To teach methods of engineering calculations of chemical processes
C5 Use of Excel spreadsheet and professional software to create simple projects and simulations

SUBJECT EDUCATIONAL EFFECTS

relating to knowledge:
PEU_W01 – knows basic technological principles
PEU_W02 - knows principles of preparing material and energy balances
PEU_W03 - knows methods to estimate physicochemical properties of a studied substance
PEU_W04 - knows basics of composition and temperature of a reacting system calculations
relating to skills:
PEU_U01 – can reach data sources about properties of a studied substance
PEU_U02 - can make simple material and energy balances and analyze them
PEU_U03 - can perform simple engineering calculations
PEU_U04 - can use professional computer software for simple engineering calculations and simulation of selected processes

PROGRAMME CONTENT

Lectures		Number of hours
Lec1	Basic terminology: technological process, chemical method concept, technological method concept. Discussion of technological principles: the principle of the best use of raw materials, the principle of the best use of energy, the principle of the best use of equipment, the principle of technological moderation. Unit operations.	2
Lec2	Material balance of the chemical process: the principle of mass conservation, the principle of atoms conservation, the principle of energy conservation. Analysis of material balance of steady-state processes. Material balance of systems with chemical reaction. The degree of conversion in the stoichiometric and non-stoichiometric mixture of reagents. Process efficiency. Process diagram, stream diagram simulation. Computer programs used to simulate chemical processes.	2
Lec3	Energy balance. Basic concepts: system state variables, system state. Principle of energy conservation, energy components of systems: internal energy, work, heat, enthalpy. Calculation of enthalpy changes. Enthalpy of reaction. The influence of temperature and pressure on the enthalpy of the reaction.	2
Lec4	Ideal gas: the equation of state, properties. Compressibility factor. Compression and expansion work . Polytropic transformation. Classification of chemical processes, types of balance sheets.	2
Lec5	Properties of chemical substances. Sources of technological information - databases. Condensed phases. Estimation of physicochemical properties: density, viscosity, critical parameters. Thermodynamic properties. Critical state of matter.	2
Lec6	Real gas. Deviations from the ideal state. Compressibility factor for real gases. Equations of real gas state. Acentric coefficient. Mixtures of real gases.	2
Lec7	Factor of gas and liquid activity. Definition of volatility and volatility coefficient. Equations for calculating volatility coefficient. Liquid activity factor. LewisRandal's rule. Phase equilibria. Functions of deviation from the ideal state.	2
Lec8	Chemical reaction. Stoichiometry; concentration, degree of conversion relative to a concentration and molar stream (change in volume). Direction of reaction; elimination of component reactions as part of the chemical process concept. Composition calculation (reaction run to the end).	2
Lec9	Composition in a state of equilibrium. Equilibrium constant. Temperature dependence of the equilibrium constant. Reactions with a change in the number of moles; pressure influence; technological treatments (excess reagent, reduction of concentration - examples). Calculation of equilibrium composition based on selected examples.	2
Lec10	Kinetic equation. Rate of an elementary reaction; concentration dependence. Irreversible and reversible elementary reactions; solving appropriate differential equations. Reaction rate constant. Change of composition over time. Rate of real reaction; full kinetic model, simplified descriptions. An approximation of the state of equilibrium and an approximation of the stationary state. Examples of complex reactions. Use of experimental data.	2
Lec11	Tank reactor. Periodic work system; perfect mixing, volume dependency on the degree of conversion and reaction time. Flow system; equation of component continuity, perfect mixing, steady state, design equation of a continuous-stirred tank reactor, conventional reaction time.	2

Lec12	Plug flow reactor. Design equation for a piston type system in a steady state. Comparison of volume and degree of conversion in continuous reactors: tank and tubular.	2
Lec13	Estimation of composition and temperature in the studied system. Heat balance. Examples. Adiabatic reaction.	2
Lec14	Written credit I	2
Lec15	Written credit II	2
	Total hours	**30**
Project		**Number of hours**
Pr1	Introduction. Basics of the used computer software. Principles of a material balance creation without chemical reaction.	2
Pr2	Simulation of selected processes - material balance without chemical reaction, process limitation.	2
Pr3	Simulation of selected processes - material balance, returned stream. Project I.	2
Pr4	Principles of material balance of processes with chemical reactions.	2
Pr5	Simulation of selected processes - material balance with parallel reactions. Project II.	2
Pr6	Projects and material overview.	2
Pr7	Written credit I.	2
Pr8	Analysis of the chemical process with regards to reaction kinetics - elementary reactions, calculations of concentrations of selected reagents, time necessary to achieve the state of equilibrium in studied systems.	2
Pr9	Analysis of the chemical process with regards to reaction kinetics - complex reactions, estimation of reaction order and kinetic parameters on the basis of experimental data.	2
Pr10	Volumetric gas properties determined from third degree real gas state equations. Project III.	2
Pr11	Volumetric gas properties determined from the Lee-Kesler real gas state equation.	2
Pr12	Functions of deviation from the ideal state: free energy, enthalpy, free enthalpy, entropy, volatility. Project IV.	2
Pr13	Influence of pressure and temperature on an equilibrium reaction process.	2
Pr14	Projects overview. Written credit II.	2
Pr15	Written credit - second term.	2
	Total hours	**30**

TEACHING TOOLS USED

N1. Lecture with multimedia presentation
N2. Excel spreadsheet
N3. Polymath computer software
N4. Computer software for simulation of chemical processes (ChemCAD or Aspen Plus)

EVALUATION OF SUBJECT LEARNING OUTCOMES ACHIEVEMENT

Evaluation (F – forming (during semester), P –	Learning outcomes number	Way of evaluating learning outcomes achievement

concluding (at semester end)		
P (lecture)	PEU_W01 – PEU_W03	Written credits I and II, exam
F1 (project)	PEU_U01 – PEU_U04	Written credit I
F2 (project)	PEU_U01 – PEU_U04	Written credit II
P (project) = (F1 + F2) / 2		

PRIMARY AND SECONDARY LITERATURE

PRIMARY LITERATURE:

[1] S. Kucharski, J. Głowiński, Podstawy obliczeń projektowych w technologii chemicznej, 3 wyd., Oficyna Wyd. PWr, Wrocław 2010

[2] J. Szarawara, J. Piotrowski, Podstawy teoretyczne technologii chemicznej, WNT, Warszawa 2010

SECONDARY LITERATURE:

[1] R.C. Reid, J.M. Prausnitz, B.E. Poling, The properties of gases and Liquids, 4th ed., Mcgraw-Hill, New York 1987

[2] Praca zbiorowa, Przykłady i zadania do przedmiotu Podstawy technologii chemicznej, Oficyna Wyd. PWr, Wrocław 1991

[3] W. Ufnalski, Wprowadzenie do termodynamiki chemicznej, Oficyna Wyd. PW, Warszawa 2004

[4] H.S. Fogler, Elements of Chemical Reaction Engineering, Fourth Ed., Prentice Hall PTR, New Jersey, 2005.

[5] D. M. Himmelblau, J. B. Riggs, Basic Principles and Calculations in Chemical Engineering, Seventh Ed., Prentice Hall PTR, New Jersey, 2004.

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