



COURSE DESCRIPTION CARD - SYLLABUS

Course name

Chemometrics and elements of statistics [N1TCh2>CiES]

Course

Field of study

Chemical Technology

Year/Semester

2/4

Area of study (specialization)

–

Profile of study

general academic

Level of study

first-cycle

Course offered in

Polish

Form of study

part-time

Requirements

compulsory

Number of hours

Lecture

20

Laboratory classes

0

Other

0

Tutorials

0

Projects/seminars

20

Number of credit points

4,00

Coordinators

dr inż. Joanna Łechtańska

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Lecturers

Prerequisites

The student should have basic knowledge of mathematics, basic chemistry and analytical chemistry. The student should have the ability to perform simple calculations and mathematical transformations. The student should have the ability to use MathCad and MS Excel computer programs. The student should understand the need for further education and increase their professional and personal competences.

Course objective

The main aim of this course is to familiarize with the basics of statistical processing of experimental data, with particular emphasis on the data obtained in the chemical laboratory.

Course-related learning outcomes

Knowledge:

1. Student has the necessary knowledge of mathematics in terms of the use of mathematical methods to describe the problems and processes of chemistry, and to perform calculations needed in engineering. [K_W01]

Skills:

1. Student can obtain necessary information from literature, databases and other sources related to chemical sciences, interpret them properly, draw conclusions, formulate and justify opinions. [K_U01]
2. Student can work both individually and in a team environment in a professional and other environment. [K_U02]
3. Student can implement the process of self-learning. [K_U05]
4. Student can use computer programs that support the tasks typical of technology and chemical engineering, plan chemical experiments, examine the course of chemical processes and properly interpret the results obtained. [K_U07]
5. Student can use mathematical knowledge to simulate, design, optimize and characterize simple chemical processes and unit operations. [K_U08]
6. Student can assess the suitability of routine methods and techniques appropriate for solving engineering tasks of a practical nature in chemical technology, can also select and apply the appropriate method and technique. [K_U14]

Social competences:

1. Student understands the need to develop and improve their professional, personal and social competences. [K_K01]
2. Student can cooperate and work on a team, inspire and integrate engineering environments. [K_K03]
3. Student can appropriately determine the priorities for accomplishing the assigned task. [K_K04]
4. Student can correctly identify problems and makes appropriate career choices, in accordance with professional ethics. [K_K05]

Methods for verifying learning outcomes and assessment criteria

Learning outcomes presented above are verified as follows:

Colloquium in the middle of the classes, passing colloquium ending the classes.

Programme content

Issues related to chemometrics and elements of statistics.

Course topics

1. Basic concepts of probability calculus:
 - Primary concepts: elementary event, elementary event space
 - Classical definition and Kolmogorov probability
 - Probability characteristics
2. Basic concepts of mathematical statistics
 - Population and sample
 - Random variables with a discrete and continuous distribution
3. Point estimation
4. Compartmental estimation
5. Verification of statistical hypotheses
6. Definition, place and role of chemometry in chemical research
7. Measurement errors
 - Division and sources of measurement errors in chemical testing
 - Error propagation
8. Uncertainty of measurement
 - Type A and B uncertainty
 - Ishikawa chart
 - Estimation of the measurement uncertainty
9. Accuracy, precision and resolution of the measuring method. Comparison of measuring methods
10. Graphical methods of research results presentation and interpretation
11. The quantities characterising the test results and their use to assess the quality of the tests
 - Position measures
 - Measures of dispersion
 - Measures of diagonality
 - Measures of flattening
12. Chemical process modelling
 - Smallest squares method

- Statistical evaluation of the model and its parameters
 - Use of models for prediction
13. Planning the experiment
- Two and three level factorial plans type 2K
 - Application of factorial plans in chemical research. Benefits and limitations.

Teaching methods

1. Lecture: a multimedia presentation illustrated with examples given on the blackboard by the teacher. In special cases, the online form of the lecture is allowed.
2. Project: a project made in the MS Excel computer program.

Bibliography

Basic:

1. D. Bobrowski, K. Łybacka, Wybrane metody wnioskowania statystycznego, Wydaw. Politechniki Poznańskiej, Poznań 2001.
2. J. Mazerski, Podstawy Chemometrii, Wydawnictwo Politechniki Gdańskiej, Gdańsk 2000.
3. J. Mazerski, Chemometria praktyczna: zinterpretuj wyniki swoich pomiarów, Malamut, 2009

Additional:

1. J.R.Taylor, Wstęp do Analizy Błędu Pomiarowego, PWN Warszawa 1999.
2. K. Mańczak, Technika Planowania Eksperymentu, WNT, Warszawa 1976.
3. J. Greń, Statystyka matematyczna modele i zadania, PWN, Warszawa 1984

Breakdown of average student's workload

	Hours	ECTS
Total workload	100	4,00
Classes requiring direct contact with the teacher	40	1,50
Student's own work (literature studies, preparation for laboratory classes/ tutorials, preparation for tests/exam, project preparation)	60	2,50