Course title: **Computer modelling in chemical technology**

Institute/Division: **FACULTY OF CHEMICAL ENGINEERING AND TECHNOLOGY**

Number of contact hours: **30 hours** (15h computer laboratories, 15h project)
Course duration: 1 semester (6th semester of regular I cycle studies - spring)
ETCS credits: **6**

Course description: The unit provides an education in solving basic chemical problems using a computing environment. The course will begin with the overview of most basic numerical methods for solving basic chemical problems, including linear and nonlinear equations and ordinary differential equations. Students will utilize the computational methods to solve wide range of chemical problems related to mass balance (steady-state, recycle, differential mass balance), chemical equilibrium (equilibrium composition for liquid phase and gas phase reactions; strong and weak electrolytes), chemical kinetics (elementary and complex reactions; kinetics models), ideal reactors (batch and semi-batch reactors, continuous stirred tank reactors), thermal effects (heat balance, non-isothermal kinetics, adiabatic batch reactor) and biochemical reaction systems (mathematical models of biomass growth, basic models of biochemical batch reactors). Students will learn from worked examples found in class and practice during implementation of computational projects. The aim is for students to learn to use basic computational software packages to solve chemical problems and to learn how to develop and analyze mathematical models of chemical systems.

Education effects :

- knowledge: Students should gain better understanding of key chemical technology concepts and should know how to solve numerical problems by computational software.
- skills: Students can use general computational software to solve basic chemical (engineering) problems. They could be able to develop, analyze and critically evaluate results of computational experiments (simulations).
- social: students will learn how to work in teams; students will develop both problem solving and critical thinking skills

Literature: [1] John Ingham, Irving J. Dunn, Elmar Heinzle, Jiri E. Prenosil and Jonathan B.Snape. Chemical Engineering Dynamics: An Introduction to Modelling and Computer Simulation. 3rd ed. Wiley-VCH, 2007. [2] David M. Himmelblau and James B. Riggs. Basic Principles and Calculations in Chemical Engineering. 7th ed. Prentice Hall, 2003. [3] Peter Atkins. Physical Chemistry. [4] Michael T. Heath. Scientific Computing - An Introductory Survey, McGraw-Hill, 1997.

Assessment method: Component grade: practical exercises (completing of small-team computational projects). Final grade is based on component grades.
Prerequisites: Basic knowledge in physical chemistry, organic and inorganic technology. Basic of computer programming (any language) could be helpful, but not obligatory.
Primary target group: Students from all specialties

Lecturer: **dr hab. inż** Szczepan Bednarz**, prof. PK**
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Deadline for application: 15th of January
Remarks: The course is regular