SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	Babeş–Bolyai University of Cluj–Napoca
1.2 Faculty	Chemistry and Chemical Engineering
1.3 Department	Chemical Engineering
1.4 Field of study	Chemical Engineering
1.5 Study cycle	Master
1.6 Study programme / Qualification	Advanced Chemical Process Engineering

2. Information regarding the discipline

2.1 Name of the discipline	**Process Modelling and Artificial Intelligence - CME7312**						
2.2 Course coordinator	Lector dr. ing. Timis Elisabeta Cristina						
2.3 Laboratory coordinator	Lector dr. ing. Timis Elisabeta Cristina						
2.4. Year of study	I	2.5 Semester	1	2.6. Type of evaluation	E	2.7 Type of discipline	DF/Compulsory

3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	4	Of which: 3.2 course	2	3.3 laboratory	2
3.4 Total hours in the curriculum	56	Of which: 3.5 course	28	3.6 laboratory	28
Time allotment:					hours
Learning using course support, bibliography, course notes					25
Additional documentation (in libraries, on electronic platforms, field documentation)					18
Preparation for laboratory, homework, papers, portfolios and essays					20
Tutorship					3
Evaluations					3

3.7 Total individual study hours	69
3.8 Total hours per semester	125
3.9 Number of ECTS credits	5

4. Prerequisites (if necessary)

4.1. curriculum	Basic science, mathematics or engineering knowledge
4.2. competencies	Basic computer using skills (Matlab)

5. Conditions (if necessary)

5.1. for the course	• The course room has to facilitate video-projection. • The course could take place online as well, employing Microsoft Teams. • Students should switch off the mobile phones during courses. • Audio and/or video recording during the course is allowed only with the approval of the course coordinator. • Students are allowed to enter and exit at the courses anytime according to their needs; the course attendance contributes to the final evaluation.
5.2. for the laboratory activities	• The laboratory room has to facilitate video-projection and the use of computers with the Matlab software installed. • The laboratory activities could take place online as well, employing Microsoft Teams, providing that all students use computers featuring the Matlab software. • Students should switch off the mobile phones during courses. • Audio and/or video recording during the seminar is allowed only after the approval of the laboratory coordinator. • Students should be present at the laboratories, as they are compulsory, according to Art. 29 of “Statutul Studentului din Universitatea Babes-Bolyai”, revised at 13.01.2013.

	• The deadline for presenting the homework/projects will be agreed between the lecturer and the students. Delays are accepted in the cases when well-founded reasons are proven. • In case of presenting the homework with delay, the grade will be penalized (0.5p/week).

6. Specific competencies acquired

Professional competencies	• Define the language and identification of advanced concepts for mathematical modelling and programming for the process engineering applications • The use of information technology techniques for data processing, modelling and simulation of chemical and biochemical processes by abstracting and representing the system in the form of mathematical models, using conventional and artificial intelligence methods • Understanding and interpreting the time and space evolution of chemical and biochemical systems by the use of modelling methods originating from biological systems and implementing the artificial intelligence instruments • Understanding and explaining the operation of the chemical process engineering equipment and installations using complex dynamic mathematical models and data processing • The development of dynamic mathematical models with lumped and distributed parameters and their implementation in simulators used for the process performance assessment in order to identify operation and control solutions for economic benefits, improved energetic efficiency and safety while reducing the negative impact on the environment • Skills to analyse systems of different types belonging to various fields of activity • Capability to adapt modelling tools to processes of different complexity and category
Transversal competencies	• Performing research and design activities in working groups or independently, using computer aided techniques and conforming to the ethical rules • The development of skills for self-evaluation of performance and self-assessment of the needs for continuous professional improvement based on permanent knowledge update related to the activity field and connected fields • The correlation of own capabilities with the labour market needs • Communicating the own points of view, in a clear and concise way, using conventional and non-conventional information technology instruments • Giving and receiving feedback with respect to professional activity

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	The development of competencies (1) to understand and explain the time and space evolution of chemical and biochemical systems, (2) to conceptualize and represent the systems in the form of mathematical models and (3) to build simulation tools to illustrate the systems real behaviour.
7.2 Specific objective of the discipline	The development of capabilities to build dynamic and steady state models for systems with lumped and distributed parameters using the analytical/numerical methods and the artificial intelligence approach.

8. Content

8.1 Course	**Teaching methods**	**Remarks**
8.1.1. Introduction to mathematical modelling. Systemic approach and modelling in process engineering. Modelling goal. Balance volumes for engineering applications. Scalar and vector fields. Intensive and extensive properties. Case studies.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; application examples
8.1.2. General formulation of the conservation principles: integral and differential form. A logical methodology to model development. Models classification. Case studies.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; applications in Matlab and COMSOL
8.1.3. Constitutive relationships used in process modelling. Transfer and reaction rates. Thermodynamics. Balance volume relations.	Lecture, explanation, conversation, exemplification,	Teaching materials: PowerPoint presentations; application examples

Equipment and control relations. Case studies.	debate	
8.1.4. Modelling lumped parameter systems (LPS). Particular form of the general conservation equation. Writing balance equations for the conservation of mass, energy and momentum.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; applications in Matlab
8.1.5. Modelling lumped parameter systems (DPS), part I. Balance volumes representation. General conservation equation for DPS. The use of microscopic balance volumes. Initial conditions. Boundary conditions. Case studies.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; applications in Matlab and COMSOL
8.1.6. Modelling DPS, part II. Classification of DPS models. The use of coupled LPS models to represent DPS. Case study.	Lecture, explanation, conversation, exemples, debate	Teaching materials: PowerPoint presentations; applications in Matlab and COMSOL
8.1.7. LPS and DPS model analysis. Analysis of ODE, DAE and PDE. Degrees of Freedom analysis, Differential Index, model stiffness.	Lecture, explanation, conversation, examples, debate	Teaching materials: PowerPoint presentations; applications in Matlab and COMSOL
8.1.8. LPS and DPS model solving. Methods for solving ODE, DAE and PDE. Analytical vs. numerical solutions. Implementation with the help of software.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; applications in Matlab and COMSOL
8.1.9. Short introduction to AI. Turing test. Milestones in the field of AI. A selection of AI techniques and applications.	Lecture, explanation, conversation, examples, debate	Teaching materials: PowerPoint presentations; AI examples and projects
8.1.10. AI sub-fields/topics to approach. Machine Learning (ML) introduction. Types of learning. ML Applications. ML in process systems engineering. Methodology.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; examples and projects
8.1.11. Artificial Neural Networks (ANNs), part 1. Neuron. ANN structures. Building ANNs. ANN learning and generalization.	Lecture, explanation, conversation, case studies, debate	Teaching materials: PowerPoint presentations; NN projects; use of online platforms
8.1.12. ANNs, part 2. Widely discussed applications of ANNs. Applications of ANNs in the field of process systems engineering. Wide spread types of ANNs and newer developments.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; NN projects; use of online platforms; NN application examples
8.1.13. Automated Reasoning. Models using fuzzy logic. Case Based Reasoning. Case studies.	Lecture, explanation, conversation, examples, debate	Teaching materials: PowerPoint presentations; application examples
8.1.14. Data mining (DM). Process engineering applications. Open-source DM software and applications.	Lecture, explanation, conversation, examples, debate	Teaching materials: PowerPoint presentations; application examples; online DM platforms

Bibliography

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19. Itti, L., 2005. Artificial Intelligence. Course at University of Southern California, http://iLab.usc.edu/classes/2005cs561
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Tennessee, Knoxville, http://web.eecs.utk.edu/~hqi/ece471-571/syllabus.htm and http://web.eecs.utk.edu/~qi/ece471-571/lecture16_nn_background.pptx

<u>Online resources</u>

- http://aima.eecs.berkeley.edu/slides-pdf/
- http://www.alanturing.net/turing_archive/pages/Reference%20Articles/TheTuringTest.html
- https://plato.stanford.edu/entries/turing-test/

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8.2 Laboratory	**Teaching methods**	**Remarks**
8.2.1. Getting knowledge on Matlab functions and s-functions. Getting knowledge on Simulink. Recap model writing and programming in Matlab, including Simulink.	coaching via dialog, application building, learning by discovery, team work	Evaluation of students' level in using the software to be employed during the practical work.
8.2.2. Write and solve functions for systems with 1 and 2 ODE. Implement in parallel in Matlab and Simulink. Compare results.	dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing and programming.
8.2.3. Application of the model development logical methodology to LPS, part I: e.g. liquid accumulation in a tank; continuous stirred tank reactor (CSTR) systems; evaporator; distillation column.	coaching via dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing and programming. Present results.
8.2.4. Application of the model development logical methodology to LPS, part II: e.g. liquid accumulation in a tank; continuous stirred tank reactor (CSTR) systems; evaporator; distillation column.	coaching via dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing and programming. Present results.
8.2.5. Application for modelling DPS, part I. The use of Matlab PDE Toolbox, pdepe solver for 1D dynamic PDE (FEM). The 1D heat transfer in a long metal rod.	dialog, application building, learning by discovery, individual and team work	Student's work (in class and at home work): course and bibliography study, model writing and implementation.
8.2.6. Application for modelling DPS, part II. The use of Matlab PDE Toolbox with GUI Interface for 2D PDE. Models of heat equation along a metal plate and along a long metal rod.	dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing and implementation.
8.2.7. Model development, calibration and verification using field data, LPS or DPS case study. Part I. Model development, implementation, solve the model with initial parameters (scalar), plot and analyse results.	dialog, application building, learning by discovery, individual work, individual and team coaching	Student's work (in class and at home work): literature study, model writing, implementation, documentation and presentation of results.
8.2.8. Model development, calibration and verification using field data, LPS or DPS case study. Part II. Parameter optimization exemplified on scalars, calibration and verification.	coaching via dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing, implementation and presentation of results.
8.2.9. Model development, calibration and verification using field data, LPS or DPS case study. Part III. Parameter optimization exemplified on dynamic series testing multiple techniques (including genetic algorithms).	coaching via dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing, implementation and presentation of results.
8.2.10. Model development, calibration and	Coaching via dialog,	Student's work (in class and at

verification using field data, LPS or DPS case study. Part IV. Calibration using the models formulated for parameters and verification.	application building, learning by discovery, individual learning, team work	home work): course and bibliography study, model writing, implementation and presentation of results.
8.2.11. Case study on parameter estimation models. ANN design, training and implementation using Neural Networks Toolbox, part I.	coaching via dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing, implementation and presentation of results.
8.2.12. Case study on parameter estimation models. ANN design, training and implementation using Neural Networks Toolbox, part II.	dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): problem solution implementation and presentation of results.
8.2.13. The implementation of a case study (it can be proposed by the students) using mathematical modelling and AI techniques exemplified during sections 8.2.1 to 8.2.12.	coaching via dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing, software implementation and presentation of results.
8.2.14. The implementation of a case study using the fuzzy logic.	coaching via dialog, application building, learning by discovery, individual learning, team work	Student's work (in class and at home work): course and bibliography study, model writing, software implementation and presentation of results.

Bibliography

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9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

- The preparation of the course content was initially performed as a result of changing opinions with professors from ETH Zurich, within the institutional partnership project "Advanced process engineering for Master and joint PhD education", IB7420-111104.
- Later changes regard newer developments in the course field and/or are related to the sustainable use of resources.
- Feedback from industry (including Azomures, Emerson, Rompetrol) has been used to comply with the expected competencies desired by potential employers.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Final examination consisting in solving a modelling and/or AI problem (steps described in a Word report and a Power Point) followed by presenting the problem and answers to questions on that specific problem. It will evaluate the way knowledge of the course has been acquired, the way of thinking, correctness and argumentation for the solutions to the problem.	Oral examination on site or online.	50%
10.5 Laboratory activities	Correctness of answers as proof of understanding and applying the knowledge taught at the laboratory and the active participation to laboratory activities.	The results of projects started in class and finished at home should be presented at the very next laboratory meeting or according to the schedule established by the coordinator together with the students.	25%
	The quality and accuracy of solving the laboratory projects/ problems/ exercises, including homework.		25%

10.6 Minimum performance standards

- The ability to apply conventional modelling methods and artificial intelligence methods to chemical and process engineering case studies (e.g. CSTR and PFR type).
- Capability to present and critically analyse own approach for solving problems.
- The use of computer and English language for continuous learning.
- 5 is the minimum average accepted for the evaluation.
- The consequence of the attempted fraud and / or plagiarism are followed by the exclusion of the student from the exam.

Date
14.04.2021

Signature of course coordinator
Timis Elisabeta-Cristina

Signature of seminar coordinator
Timis Elisabeta-Cristina

Date of approval

April 25, 2021

Signature of the Director of the Department

Prof. dr. ing. Graziella Liana Turdean