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. eng. Timis Elisabeta Cristina						
2.3 Laboratory coordinator	Lector dr. eng. 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 must facilitate video-projection. • The course could take place online as well, employing Microsoft Teams. • Students must switch off the mobile phones during courses. • Audio and/or video recording during the course is not allowed. • Students are allowed to enter and exit at the courses anytime according to their needs; the active participation in courses contributes to the final evaluation.
5.2. for the laboratory activities	• The laboratory room must facilitate video-projection and the use of computers with MATLAB installed. • The laboratory activities could take place online as well, employing Microsoft Teams, providing all students use computers featuring MATLAB. • Students should switch off the mobile phones during courses. • Audio and/or video recording during the laboratory is not allowed. • 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 and tasks will be posted as Microsoft Teams Assignments. Delays are

	accepted in the cases when well-founded reasons are proven before the deadline. • 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 concepts for mathematical modelling and programming for the process engineering applications. • 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. • The use of information technology techniques for data processing, modelling and simulation of chemical and biochemical processes using conventional and artificial intelligence methods. • Understanding and interpreting the time and space evolution of chemical and biochemical systems using modelling methods originating from practical systems and implementing the artificial intelligence instruments. • Understanding and explaining the operation of chemical process engineering equipment and installations using dynamic mathematical models and data processing. • The development of dynamic mathematical models for systems with lumped and distributed parameters and their implementation in simulators used for process performance assessment to identify operation and control solutions for economic benefits, improved energetic efficiency and safety while reducing the negative impact on the environment.
Transversal competencies	• Performing research and design activities in working groups or independently, using computer aided techniques and conforming to ethical rules. • The development of skills for self-evaluation of performance and self-assessment of 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 own points of view clear and concisely 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 systems in the form of mathematical models and (3) to build simulation tools to illustrate the systems behaviour.
7.2 Specific objective of the discipline	The development of capabilities to build, optimize and validate 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. Equipment and control relations. Case studies.	Lecture, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; application examples

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. Widespread 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

1. Timis, E.C., 2023, Process Modelling and Artificial Intelligence: Microsoft PowerPoint slide show performed during course classes.
2. CAPE Centre, University of Queensland, Hungarian Academy of Sciences, 2013. Course CHEE3007: Process modelling and dynamics, available online: https://www.coursehero.com/sitemap/schools/2697-Queensland/courses/9008835-CHEE3007/, accessed on 02.04.2020.
3. Hangos K.M., Cameron I.T., 2001, Process Modelling and Model Analysis, Volume 4, 1st Edition, Academic Press, pp. 543.
4. Russell, S., Norvig, P., 2009. Artificial Intelligence: A Modern Approach 3rd edition [AIMA], Prentice-Hall, http://aima.eecs.berkeley.edu/slides-pdf/

Additional Bibliography

5. Agachi, P.S., Cristea, V.M., 2014. Basic Process Engineering Control. Berlin, Boston: De Gruyter.
6. Agachi, P.S., Cristea, V.M., Csavdari, A., Szilagyi, B., 2016. Advanced Process Engineering Control. Berlin, Boston: De Gruyter.
7. Agachi, P.S., Nagy, Z.K., Cristea, V.M., Imre-Lucaci, A., 2006, *Model Based Control - Case Studies in*

Process Engineering, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.
8. Al Aani, S., Bonny, T., Hasan, S.W., Hilal, N., 2019, Can machine language and artificial intelligence revolutionize process automation for water treatment and desalination? Desalination, 258, 84-96.
9. Andasari, V. 2015. Numerical Methods and Modeling in Biomedical Engineering, Course at Boston University, http://people.bu.edu/andasari/courses/Fall2015/be503703Fall2015.html
10. Ani, E.C., 2009. Minimization of the experimental workload for the prediction of pollutants propagation in rivers. Mathematical modelling and knowledge re-use. Acta Universitatis Lappeenrantaensis 355, Lappeenrannan teknillinen yliopisto, Digipaino, Lappeenranta, Finland, pp. 189, available online: http://urn.fi/URN:ISBN:978-952-214-830-8.
11. Bagheri, M., Akbari, A., Mirbagheri, S.A., 2019. Advanced control of membrane fouling in filtration systems using artificial intelligence and machine learning techniques: A critical review, Process Safety and Environmental Protection, 123, 229-252.
12. Darmiana, M.D., Monfareda, S.A.H., Azizyana, G., Snyderb, S.A., Giesyd, J.P., 2018. Assessment of tools for protection of quality of water: Uncontrollable discharges of pollutants, Ecotoxicology and Environmental Safety, 161, 190–197.
13. Dincer I., Ezan M.A., 2018. Fundamental Aspects of Thermodynamics and Heat Transfer. In: Heat Storage: A Unique Solution for Energy Systems. Green Energy and Technology. Springer, Cham, 1-34.
14. Califf, M.E., 2010. Introduction to Artificial Intelligence, ITK 340, Course at Illinois State University.
15. Ceccaroni, L., 2008, Artificial Intelligence Introduction, Course at Universidad Politecnica de Cataluna.
16. desJardins, M., 2005. Principles of Artificial Intelligence. Course at University of Maryland, Baltimore, http://www.cs.umbc.edu/courses/graduate/671/fall05/slides/c1_intro.ppt
17. Finn, T., 2016. Introduction to Artificial Intelligence, Course at University of Maryland, Baltimore, https://www.csee.umbc.edu/courses/undergraduate/471/spring19/01/notes/01_introduction/01.pdf
18. Howard, P., 2005. Partial Differential Equations in MATLAB 7.0. Lecture Notes. Course at Texas A&M University, http://www.tem.uoc.gr/~marina/pdemat.pdf and also https://www.math.tamu.edu/~phoward/
19. Itti, L., 2005. Artificial Intelligence. Course at University of Southern California, http://iLab.usc.edu/classes/2005cs561
20. Ismini, L., 2017. Introduction to Deep Learning, http://times.cs.uiuc.edu/course/510f17/ppt/deep-learning.pptx, part of Zhai, Z.X., 2017, Advanced Information Retrieval, Course at University of Illinois at Urbana-Champaign, http://times.cs.uiuc.edu/course/510f17/schedule.html
21. Liu, Y., Zhao, T., Ju, W., Shi, S., 2017. Materials discovery and design using machine learning, Journal of Materiomics, 3, 3, 159-177.
22. Maclin, R., 2001. Machine Learning, Course at University of Minnesota Duluth, https://www.d.umn.edu/~rmaclin/cs5751/index.html, text after Mitchell T., 1997, *Machine Learning*, McGraw Hill.
23. Maloof, M., 2017, Articial Intelligence: An Introduction, Course at Georgetown University.
24. Matuszek, P., 2010. Artificial Intelligence. Introduction and Intelligent Agents. Course at Villanova University, Philadelphia.
25. Pokutta, S., 2016. Machine Learning in Engineering Applications and Trends, NASA Workshop Machine Learning Technologies and Their Applications to Scientific and Engineering Domains Workshop, http://www.nianet.org/wp-content/uploads/2016/06/Pokutta_20160816_NASA.pdf
26. Sipos, A., Cristea, V.M., Mudura, E., Imre-Lucaci, A., Bratfalean, D., 2014, Modelarea, simularea si conducerea avansată a bioproceselor fermentative, Vol. II. Editura Universităţii “Lucian Blaga”, Sibiu.
27. Subasi, A., 2011-2012, Machine Learning Course Introduction, International Burch University.
28. Visa, A., 2005. Neural Computation Introduction. Course at Tampere University of Applied Sciences, available online: http://www.cs.tut.fi/~avisa/2806nn1.ppt
29. Wei, J., Chu, X., Sun, X.Y, Xu, K., Deng, H.X., Chen, J., Wei, Z., Lei, M., 2019. Machine learning in materials science, InfoMat, 1, 338–358.
30. Welling, 2007. Introduction to AI, Course at University of California, Irvine, available online: http://www.ics.uci.edu/~welling/teaching/ICS171spring07/ICS171spring07.html
31. Yanikoglu, B., 2017. Machine Learning, Course at Sabanci University, Turkey, http://people.sabanciuniv.edu/berrin/cs512/lectures/ (1-ml-ch1-intro.pdf and 7-nn1-intro.ppt.pdf)
32. Zabihi, R., Mowla, D., Karami, H.R., 2019, Artificial intelligence approach to predict drag reduction in crudeoil Pipelines, Journal of Petroleum Science and Engineering 178, 586–593.
33. Zhang, Z., Qi, H., 2018. Neural Network Background, in Pattern Recognition, Course at University of 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

Online resources

- 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/

Note: titles of the bibliography items may be found at one of the following: (1) the Library of the Chemical Engineering Department; (2) the Library of the Faculty of Chemistry and Chemical Engineering Faculty; (3) the "Lucian Blaga" Central Library of Babes-Bolyai University; (4) online on the Science Direct database available from the intranet of Babes-Bolyai University and "Lucian Blaga" Central Library; (5) online using specified links.

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, teamwork	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, teamwork	Student's work in class and at home: 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.	coaching via dialog, application building, learning by discovery, individual learning, teamwork	Student's work in class and at home: 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	coaching via dialog, application building, learning by discovery, individual learning, teamwork	Student's work in class and at home: 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. 1D modelling of a system with 2 output variables.	dialog, application building, learning by discovery, individual and teamwork	Student's work in class and at home: 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, teamwork	Student's work in class and at home: 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: 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, teamwork	Student's work in class and at home: 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 AI).	coaching via dialog, application building, learning by discovery, individual learning, teamwork	Student's work in class and at home: 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, teamwork	home: 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, teamwork	Student's work in class and at home: 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, teamwork	Student's work in class and at home: problem solution implementation and presentation of results.
8.2.13. The implementation of a case study (it can be proposed by students) using mathematical modelling, AI techniques exemplified during sections 8.2.1 to 8.2.12. Or the exemplification of a model employed for industrial process simulation and control using Mimic and/or DeltaV.	coaching via dialog, application building, learning by discovery, individual learning, teamwork	Student's work in class and at home: course and bibliography study, model writing, 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, teamwork	Student's work in class and at home: course and bibliography study, model writing, implementation and presentation of results.

Bibliography

1. All course bibliography
2. Berk, Z., 2009. Chapter 21 - Evaporation, In Food Science and Technology, Food Process Engineering and Technology, Academic Press, 429-458.
3. Glover, W.B., 2004. Chemical Engineering Progress, AIChE, December 2004, 26-33, https://lcicorp.com/test_design/selecting_evaporators_for_process_applications/
4. Sipos, A., Cristea, V.M., Mudura, E., Imre Lucaci A., Bratfalean, D., 2014. Modelarea, simularea si conducerea avansată a bioproceselor fermentative, carte de specialitate; Editura Universităţii "Lucian Blaga" din Sibiu; Vol. II.
5. Xue, D., Chen Y., 2009. Solving applied mathematical problems with MATLAB. Chapman & Hall/CRC, Boca Raton, USA.
6. Partial Differential Toolbox, Matlab, User Guide.
7. COMSOL Mutiphysiscs 3.1, UserGuide.
8. Neural Network Toolbox, Matlab, User Guide.
9. Fuzzy Logic Toolbox, Matlab, UserGuide.

Note: titles of the bibliography items may be found at one of the following: (1) the Library of the Chemical Engineering Department; (2) the Library of the Faculty of Chemistry and Chemical Engineering Faculty; (3) the "Lucian Blaga" Central Library of Babes-Bolyai University; (4) online on the Science Direct database available from the intranet of Babes-Bolyai University and "Lucian Blaga" Central Library; (5) online using specified links.

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 course content preparation was initially performed by 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 development.
- Feedback from industry (including Azomures, Emerson, and Rompetrol) has been used to comply with expected competencies desired by potential employers.
- The competencies and qualifications have been set in accordance to the Diploma Supplement and qualifications of the National Authority of Qualifications standards

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 doc or pdf report according to instructions provided, a Power Point presentation and the model files as implemented in the specific software) 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	50%
10.5 Laboratory activities	Correctness of answers as proof of understanding and applying the knowledge taught during laboratory and the active participation to laboratory activities.	The results of homework and projects started in class and finished at home must be presented according to the specific agreed schedule.	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, biochemical and process engineering case studies (e.g. CSTR and PFR type).
- The capacity to write mathematical models in MATLAB.
- Capability to present and critically analyse own approach for solving mathematical modelling and AI problems.
- The use of computer and English language for continuous learning.
- 5 is the minimum grade accepted to pass the evaluation.
- The consequence of the attempted fraud and / or plagiarism are followed by the exclusion of the student from the exam.

Date
07.04.2023

Signature of course coordinator
Timis Elisabeta Cristina

Signature of laboratory coordinator
Timis Elisabeta Cristina

Date of approval

25.04.2023

Signature of the Director of the Department

....