SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	Babeş–Bolyai Universitaty 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	Conf. dr. ing. Cristea Vasile Mircea						
2.3 Seminar coordinator	Conf. dr. ing. Cristea Vasile Mircea						
2.4. Year of study	I	2.5 Semester	1	2.6. Type of evaluation	E	2.7 Type of discipline	Compulsory

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

3.1 Hours per week	3	Of which: 3.2 course	2	3.3 seminar/laboratory	1
3.4 Total hours in the curriculum	42	Of which: 3.5 course	28	3.6 seminar/laboratory	14

Time allotment:	hours
Learning using manual, course support, bibliography, course notes	40
Additional documentation (in libraries, on electronic platforms, field documentation)	30
Preparation for seminars/labs, homework, papers, portfolios and essays	30
Tutorship	3
Evaluations	3
Other activities:	

3.7 Total individual study hours	108
3.8 Total hours per semester	150
3.9 Number of ECTS credits	6

4. Prerequisites (if necessary)

4.1. curriculum	• Basic science, mathematics or engineering knowledge
4.2. competencies	• Basic computer using skills

5. Conditions (if necessary)

5.1. for the course	• Students should switch off the mobile phones during courses and seminars. • Students should be present at the courses without any time delay.
5.2. for the seminar /lab	• The deadline for presenting the homework results will be agreed

activities	between the seminar holder and the students. No delay is accepted for the presentation of the homework results unless well-founded reasons are proven. • In case of presenting the homework with delay, the grade will be penalized by 0.5 points/ week of delay. • Students should be present at the seminars without any time delay.

6. Specific competencies acquired

Professional competencies	• Defining the language and identification of advanced concepts for mathematical modelling and programming for the process engineering applications • Understanding and explaining the operation of the chemical process engineering equipment and installations using complex dynamic mathematical models and statistical data processing • Development of competencies of using information technology techniques for data processing, modelling and simulation of chemical and biochemical processes by abstracting and representing the system in the form of a mathematical models, using conventional and artificial intelligence methods • Developing the competencies for understanding and interpreting the time and space evolution of the chemical and biochemical system by the use of modelling methods originating from the biological systems and implementing the artificial intelligence instruments. • Developing 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
Transversal competencies	• Performing research and design activities in a autonomous way, using computer aided techniques and conforming to the ethical rules • Developing of self guided evaluation of own professional performance and self assessment of the needs for continuous professional improvement based on permanent knowledge update related to his/her activity field • Communicating the own points of view, in a clear and concise way, using communication means based on conventional and non-conventional information technology instruments

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

7.1 General objective of the discipline	• Developing the competencies of understanding and interpretation of the for time and space evolution of the chemical and biochemical system, abstracting and representing the system in the form of a mathematical model and building software simulators to illustrate the real system behaviour
7.2 Specific objective of the discipline	• Developing the capability of building dynamic/stationary models for systems with lumped/distributed parameters using both the first principle and the artificial instruments approach

8. Content

8.1 Course	Teaching methods	Remarks
8.1.1. Thermodynamic principles used in process modelling. Scalar and vector fields. Intensive and extensive thermodynamic properties. Degrees of freedom.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL

		application examples
8.1.2. General formulation of the conservation principles (laws) both in integral and differential form. Balance volumes used in process system applications. Constitutive relationships used in process modelling.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.3. Total and component mass conservation balances, energy conservation balance and momentum conservation balance for processes with lumped parameters (PLP) (I).	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.4. Total and component mass conservation balances, energy conservation balance and momentum conservation balance for processes with lumped parameters (PLP) (II). Coupled Differential and Algebraic Equations (DAE).	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.5. DAE Index. Normalization of the DAE. Stability of the DAE. Stiff DAE. Numerical solutions of the differential equations and DAE.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.6. Modelling processes with distributed parameters (PDP). Balance volumes. Initial conditions. Boundary conditions. Dirichlet, Neumann and Robbin boundary conditions.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.7. Non-dimensional forms of the of the PDE for the PDP models. Classification of the PDP models: parabolic, hyperbolic and elliptic forms. PLP models used for representing PDP.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.8. Methods for solving PDE. Finite difference methods for solving parabolic equations, Crank-Nicholson method. Solving elliptic equations. Orthogonal collocation. FEM.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.9. Statistical modeling using artificial neural networks (ANN). Natural and artificial neuron. Perceptron.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.10. Multilayer ANNs. Supervised and unsupervised learning. Linear ANNs.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples

8.1.11. Feedforward ANN and the backpropagation training algorithm.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.12. Radial Basis and probabilistic ANN, Self organizing maps, prediction and classification using ANN.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.13. Models using fuzzy logic.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples
8.1.14. Mathematical models for process fault diagnosis and control.	Lecture giving, explanation, conversation, exemplification, debate	Teaching materials: PowerPoint presentations; Matlab, Simulink, NN Toolbox and COMSOL application examples

Bibliography

1. Katalin Hangos, Ian Cameron, *Process Modelling and Model Analysis*, Academic Press, 2001.
2. J. Ingham, I.J. Dunn, E. Heinzle, J.E. Prenosil, J.B. Snape, *Chemical Engineering Dynamics,* Wiley-VCH, 2007.
3. Simon Haykin, *Neural Networks* A Comprehensive Foundation, Mcmillan Publishing Company, Englewood Cliffs, NJ 07632, 1994.
4. Paul Serban Agachi, Zoltan K. Nagy, Mircea Vasile Cristea, Arpad Imre-Lucaci, *Model Based Control - Case Studies in Process Engineering*, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2006.
5. V. M. Cristea, V. Marinoiu, S. P. Agachi, *Reglarea predictivă după model a instalației de cracare catalitică*, Editura Casa Cărții de Știință, 2003.

Note: titles of the bibliography items may be found at the Library of the Chemical Engineering and Oxide Materials Chair, at the Faculty of Chemistry and Chemical Engineering Faculty, branch of the "Lucian Blaga" Central Library of Babes-Bolyai University and at the Library of the Technical University of Cluj-Napoca.

8.2 Seminar / laboratory	Teaching methods	Remarks
8.2.1. Applications for PLP modelling: liquid accumulation tank, continuous stirred tank reactor, evaporator, distillation column, alcoholic fermentation bioreactor; normalization of the differential equations.	Conversation method, learning by discovery, individual learning, team working, application building	*Student's work*: course and literature study (bibliography), recapitulating Matlab and Simulink programming.
8.2.2. Application for complex modelling of PLP: Activated Sludge Waste Water Treatment Plant including organic compounds and nitrogen removal (aerated reactors anoxic reactors and settler), The ASM1 model.	Conversation method, learning by discovery, individual learning, team working, application building	*Student's work*: course and literature study (bibliography), solving the homework (project).
8.2.3. Application for modelling PDP: tubular heat exchanger. Application for 3D heat transfer. Application for river pollution.	Conversation method, learning by discovery, individual learning, team working, application building	*Student's work*: course and literature study (bibliography), individual study, team study, solving the

		homework (project).
8.2.4. Getting knowledge on *Partial Differential Toolbox* of Matlab. Getting knowledge on COMSOL Multiphysics (based on Finite Element Method) for simulating PDP processes- General Form.	Conversation method, learning by discovery, individual learning, team working, application building	*Student's work*: course and literature study (bibliography), individual study, solving the homework (project).
8.2.5. ANN design, training and implementation using Neural Networks Toolbox (NNT), Feedforward backpropagation. Radial basis and probabilistic ANN.	Conversation method, learning by discovery, individual learning, team working, application building	*Student's work*: course and literature study (bibliography), individual study, team study, solving the homework (project).
8.2.6. Application for modelling the Fluid Catalytic Cracking Unit using Artificial Neural Networks and Fuzzy Logic. Classification of different sorts of teas using ANN.	Conversation method, learning by discovery, individual learning, team working, application building	*Student's work*: course and literature study (bibliography), individual study, solving the homework (project).
8.2.7. Application for modelling PDP: sodium carbonate production in a rortary calcinatory. Application for the control of the hexamethylene reactor using fuzzy logic.	Conversation method, learning by discovery, individual learning, team working, application building	*Student's work*: course and literature study (bibliography), individual study, solving the homework (project).

Bibliography

1. Katalin Hangos, Ian Cameron, *Process Modelling and Model Analysis*, Academic Press, 2001.
2. J. Ingham, I.J. Dunn, E. Heinzle, J.E. Prenosil, J.B. Snape, *Chemical Engineering Dynamics*, Wiley-VCH, 2007.
3. *Partial Differential Toolbox*, Matlab, User Guide.
4. *COMSOL Mutiphysiscs 3.1*, UserGuide.
5. *Neural Network Toolbox*, Matlab, User Guide.
6. *Fuzzy Logic Toolbox, Matlab*, UserGuide.

Note: titles of the bibliography items may be found at the Library of the Chemical Engineering and Oxide Materials Chair, at the Faculty of Chemistry and Chemical Engineering Faculty, branch of the "Lucian Blaga" Central Library of Babes-Bolyai University and at the Library of the Technical University of Cluj-Napoca.

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 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.
- Feedback from industry (Companies: Azomureş, Oltchim, ChimComplex) 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 a written work which will evaluate the way knowledge of the course has been acquired, the way of thinking, correctness and argumentation for the solutions to the examination subjects	Written examination. Access to examination is conditioned by the presentation of the homework solutions. Examination fraud: the student is expelled from the exam according the ECTS regulations	50%
10.5 Seminar/lab activities	Correctness of the answers as proof of: understanding and applying the knowledge taught at the seminar/laboratory, active participation to the seminar/laboratory activities	The solutions of the homework problems should be presented at the very next laboratory/seminar meeting	10%
	The quality and accuracy of solving the homework problems		40%
10.6 Minimum performance standards			
• Ability to apply modelling and artificial intelligence engineering tools to engineering practice cases (CSTR and PFR cases); design of experiments and projects using computed aided engineering tools (CSTR and PFR cases). • Capability to critically analyse own approach for solving problems; use computer and English language for continuous learning.			

Date

5.05.2014

Signature of course coordinator

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Signature of seminar coordinator

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Date of approval

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Signature of the head of department

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