SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	Babeş-Bolyai University
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 / Master's degree in Chemical Engineering

2. Information regarding the discipline

2.1 Name of the discipline	**Advanced Physical Chemistry – CME6111**						
2.2 Course coordinator	Prof. Dr. Liana Mureşan (Electrochemistry „EC") Assoc. Prof. Dr. Eng. Adrian Nicoara (Thermodynamics „TD") Lect. Dr. Dana-Maria Sabou (Chemical Kinetics "CK")						
2.3 Seminar coordinator	Prof. Dr. Liana Mureşan (Electrochemistry „EC") Assoc. Prof. Dr. Eng. Adrian Nicoara (Thermodynamics „TD") Lect. Dr. Dana-Maria Sabou (Chemical Kinetics "CK")						
2.4. Year of study	I	2.5 Semester	1	2.6. Type of evaluation	E	2.7 Type of discipline	Mandatory

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

3.1 Hours per week	4	Of which: 3.2 course	2	3.3 seminar	2
3.4 Total hours in the curriculum	56	Of which: 3.5 course	28	3.6 seminar	28
Time allotment:					hours
Learning using manual, course support, bibliography, course notes					26
Additional documentation (in libraries, on electronic platforms, field documentation)					18
Preparation for seminars/labs, homework, papers, portfolios and essays					20
Tutorship					2
Evaluations					3
Other activities: not the case					-

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	• Not the case
4.2. competencies	• Not the case

5. Conditions (if necessary)

5.1. for the course	• The students will turn off their mobile phones

	• Delays will not be tolerated
5.2. for the seminar /lab activities	• Students will attend the seminar with information of the course notes corresponding to the current seminar topic and, when required, will bring their personal laptop • Students will turn off their mobile phones • Delays will not be tolerated

- Descrierea, analiza şi utilizarea conceptelor şi teoriilor avansate din domeniul chimiei şi ingineriei chimice de proces.

6. Specific competencies acquired

Professional competencies	• Description, analysis and use of the concepts and theories from the field of chemistry and chemical process engineering. • Definition of notions, concepts, theories and advanced models in the field of chemistry and chemical process engineering as well as their adequate use within the professional community. • Use of advanced knowledge in the field of chemistry and chemical process engineering to explain and interpret chemical processes. • Identification and proper usage of concepts, method and theories for solving new complex problems of chemical process engineering. • Critical analysis and usage of principles, methods and advanced work techniques for quantitative and qualitative evaluation of chemical process engineering.
Transversal competencies	• Independent execution of complex professional duties and research projects using computer-aided techniques and comply with professional ethics and moral. • Planning, monitoring and assuming professional duties of underline group. Proving the coordination capabilities, analytical thinking, adaptability and flexibility, collaboration with team members. • Auto-evaluation of professional performances and establish the needs of continuous learning, documentation in the work fields in correlation with the labour market.

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

7.1 General objective of the discipline	• Approach of advanced concepts of physical chemistry (thermodynamics, chemical kinetics, electrochemistry).
7.2 Specific objective of the discipline	• Advanced approach in the field of thermodynamics of open systems and of irreversible processes; study of the thermodynamics of heterogeneous phase equilibrium. • Correlation of advanced thermodynamics fundamentals and the ability to use / apply / correlate theoretical knowledge and interpret phenomena and processes associated in the field. • Interpretation of kinetic data from the point of view of rate laws and reaction mechanisms. • Detailed approach to dealing with rate laws and mechanisms of some classes of reactions with practical applications (enzymatic reactions, redox reactions). • Approach of advanced concepts of electrochemistry: the electric double layer; electro-capillary and electro-kinetic phenomena; types of overpotential; reactions under mixed control (activation + diffusion); The Marcus Theory • Training of students to use electrochemical investigation methods for the electrode processes; Cyclic voltammetry.

8. Content

8.1 Course	Teaching methods	Remarks
8.1.1. TD1: Review of the main consequences of first and second laws of thermodynamics.	Presentation; Explanation, Conversation; Description; Debate	
8.1.2. TC2: Second law consequences. Reaction entrophy. Affinity. Spontaneity of chemical processes.	Presentation; Explanation, Conversation; Description; Debate	
8.1.3. TD2: Introduction in irreversible processes thermodynamics. Basic concepts. Local equilibrium hypostesis. Entropy balance.	Presentation; Explanation, Conversation; Description; Debate	
8.1.4. TD3: General theory of irreversible process thermodynamics: 7 steps formulation.	Presentation; Explanation, Conversation; Description; Debate	
8.1.5. TD4: Minimum entropy production principle. Application to heat a mass transport.	Presentation; Explanation, Conversation; Description; Debate	
8.1.6. CK1: Recap of fundamental concepts in chemical kinetics. Experimental approaches in chemical kinetics.	Presentation (PPT); Explanation, Conversation; Description; Debate	
8.1.7. CK2: Processing kinetic experimental data: determination of reaction orders and rate coefficients. Empirical rate laws.	Presentation (PPT); Explanation, Conversation; Description; Debate	
8.1.8. CK3: Interpretation of the empirical rate laws from the point of view of reaction mechanisms.	Presentation (PPT); Explanation, Conversation; Description; Debate	
8.1.9. CK4: Rate laws and mechanisms in enzymatic reactions.	Presentation (PPT); Explanation, Conversation; Description; Debate	
8.1.10. CK5: Rate laws and mechanisms in redox reactions.	Presentation (PPT); Explanation, Conversation; Description; Debate	
8.1.11. EC1: Recap of fundamental concepts in electrochemistry. The electric double layer.	Presentation; Explanation, Conversation; Description; Debate	
8.1.12. EC2: Types of overpotentials. Electrolysis. Advanced electrochemical kinetics.	Presentation; Explanation, Conversation; Description; Debate	
8.1.13. EC3: Electrochemical obtaining methods.	Presentation; Explanation, Conversation; Description; Debate	
8.1.14. EC4: Electrochemical investigation methods of electrode processes (classification, examples) and cyclic voltammetry.	Presentation; Explanation, Conversation; Description; Debate	

Bibliography

1. G. Lebon, Understanding Non-equilibrium Thermodynamics, Springer-Verlag, Berlin, 2008.
2. P.W. Atkins, "Tratat de chimie fizică", Ed. Tehnică, 1996.
3. I.G. Murgulescu, R. Valcu, "Introducere în chimia fizică. Termodinamica chimică", vol III, Ed. Academiei RSR, Bucureşti, 1982.
4. I. Bâldea, „Deducerea mecanismului de reacţie", Presa Universitară Clujeană, Cluj-Napoca, 2008.
5. I. Bâldea, „Cinetică chimică şi mecanisme de reacţie. Baze teoretice şi aplicaţii", Presa Universitară Clujeană, Cluj-Napoca, 2002.
6. I. Bâldea, „Some Advanced Topics in Chemical Kinetics", Cluj University Press, Cluj-Napoca, 2000.
7. L. Oniciu, E. Constantinescu, „Electrochimie şi coroziune", Editura Didactică şi Pedagogică, Bucureşti, 1987.
8. L. Oniciu, L. Mureşan, „Electrochimie aplicată", Presa Universitară Clujeană, Cluj-Napoca, 1998.

8.2 Seminar	Teaching methods	Remarks
8.2.1. TD1: Heat of reaction for isothermal processes.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.2. TD2: Heat of reaction for adiabatical processes.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.3. TD3: Numerical applications of second law of	Explanation, Conversation;	

thermodynamics.	Description; Debate; Problem solving	
8.2.4. TD4: Numerical applications of irreversible processes thermodynamics: heat transfer/transport.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.5. TD5: Numerical applications of irreversible processes thermodynamics: mass transfer/transport.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.6. CK1: Numerical applications of fundamental concepts in chemical kinetics. Experimental approaches in chemical kinetics – case studies.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.7. CK2: Determination of partial reaction orders and individual rate coefficients from experimental data. Expression of empirical rate laws. *(numerical applications provided to the students electronically, to be solved by the use of suitable software)*	Explanation, Conversation; Description; Debate; Problem solving (using suitable software)	
8.2.8. CK3: Interpretation of experimental rate laws from the point of view of reaction mechanism. *(numerical applications provided to the students electronically, to be solved by the use of suitable software)*	Explanation, Conversation; Description; Debate; Problem solving (using suitable software)	
8.2.9. CK4: Interpretation of experimental data of enzymatic reactions in the absence and in the presence of modifiers (activators / inhibitors). *(numerical applications provided to the students electronically, to be solved by the use of suitable software)*	Explanation, Conversation; Description; Debate; Problem solving (using suitable software)	
8.2.10. CK5: Interepretation of experimental data of redox reactions. *(numerical applications provided to the students electronically, to be solved by the use of suitable software)*	Explanation, Conversation; Description; Debate; Problem solving (using suitable software)	
8.2.11. EC1: Numerical applications of fundamental concepts in electrochemistry.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.12. EC2: Numerical applications of advanced electrochemical kinetics (I).	Explanation, Conversation Debate; Problem solving	
8.2.13. EC3: Numerical applications of advanced electrochemical kinetics (II).	Explanation, Conversation; Description; Debate; Problem solving	
8.2.14. EC4: Various calculations and applications to the concepts discussed within the other lectures.	Explanation, Conversation; Description; Debate; Problem solving	

Bibliography

1. P.W. Atkins, J. De Paula, "Chimie Fizica", Ed. AGIR, 2003.
2. H. E. Avery, D. J. Shaw, "Basic Physical Chemistry Calculations", Butterworth & Co., 1980.
3. I. Baldea, „Cinetica Chimica si mecanisme de reactie. Baze teoretice si aplicatii", Presa Universitara Clujeana, Cluj-Napoca, 2002**.**
4. Experimental data (provided at the appropriate time).
5. G. Niac, V. Voiculescu, I. Baldea, M. Preda, „Formule tabele probleme de chimie fizică", Editura Dacia, Cluj-Napoca, 1984.
6. Notes provided by lecturers.

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

- By instructing the theoretical and practical concepts of **Advanced Physical Chemistry** course, the students will get the knowledge in accordance with the competencies requested by possible employment sectors stetted by RNCIS.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Correctness of answers – proper understanding and learning of concepts discussed during lectures; Correct use of learned concept within new contexts. Correct solving of problems as inherent part of examination subjects.	Written colloquia consisting of three sets of subjects corresponding to the TC, CC and EC modules of the course. Proven or intended fraud is punished according to the ECST rules of UBB.	100 % (Each module contributes to the final mark with one third that is with 33.3 %)
10.5 Seminar/lab activities	Correctness of answers – proper understanding and learning of concepts discussed during seminars; Correct use of learned concept within new contexts.	Evaluated by means of problems to be solved, as inherent part of the examination subjects.	-
10.6 Minimum performance standards			

- Grade 5 (five) at the written colloquia, at each of the three separate modules of the course (TC, CC and EC).
- Adequate knowledge and usage of basic concepts of advanced physical chemistry.

Date	Signature of course coordinator	Signature of seminar coordinator
23.02.2018	Prof. Dr. Liana Mureşan	Prof. Dr. Liana Mureşan
	Assoc. Prof. Dr. Eng. Adrian Nicoară	Assoc. Prof. Dr. Eng. Adrian Nicoară
	Lect. Dr. Dana-Maria Sabou	Lect. Dr. Dana-Maria Sabou

Date of approval

Signature of the head of department

Conf. Dr. Ing. Graziella Liana Turdean

26 februarie 2018