SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	Babes-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

2. Information regarding the discipline

2.1 Name of the discipline	**Advanced Physical Chemistry – CME6111**						
2.2 Course coordinator	Assoc. Prof. Dr. Eng. Graziella Liana Turdean (Thermodynamics „TD”) Prof. Dr. Liana Mureşan (Electrochemistry „EC”) Assoc. Prof. Dr. Eng. Alexandra Csavdári (Chemical Kinetics “CK”)						
2.3 Seminar / laboratory work coordinator	Assoc. Prof. Dr. Eng. Graziella Liana Turdean (Thermodynamics „TD”) Prof. Dr. Liana Mureşan (Electrochemistry „EC”) Assoc. Prof. Dr. Eng. Alexandra Csavdári (Chemical Kinetics “CK”)						
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	0/1
3.4 Total hours in the curriculum	42	Of which: 3.5 course	28	3.6 seminar/laboratory	0/14

Time allotment:	hours
Learning using manual, course support, bibliography, course notes	42
Additional documentation (in libraries, on electronic platforms, field documentation)	9
Preparation for seminars/labs, homework, papers, portfolios and essays	42
Tutorship	12
Evaluations	3
Other activities: not the case	-

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	• 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 bring to the laboratory practice their course notes and appropriate calculus device • Students will turn off their mobile phones • Delays will not be tolerated

6. Specific competencies acquired

Professional competencies	• 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. • Interpretation of kinetic data for complex reaction systems. • 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 concepts of chemical thermodynamics.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.2. TD2: Thermodynamics of open systems.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.3. TD3: Phase equilibrium in heterogeneous systems.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.4. TD4: Thermodynamics of irreversible process.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.5. CK1: Recap of fundamental concepts in chemical kinetics and the bond to applications in chemical engineering.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.6. CK2: Processing kinetic experimental data – general concepts, determination of reaction orders and rate coefficients. Empirical rate laws.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.7. CK3: Interpretation of rate laws from the point of view of reaction mechanisms.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.8. CK4: Methods of obtaining experimental data and their interpretation to determine the rate determining step.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.9. CK5: Determination of individual rate coefficient for some complex reaction systems.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.10. EC1: Recap of fundamental concepts in electrochemistry. The electric double layer.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.11. EC2: The Marcus Theory. Types of overpotential.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.12. EC3: Advanced electrochemical kinetics.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.13. EC4: Electrochemical investigation methods of electrode processes (classification, examples) and cyclic voltammetry.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.14. Calculus examples for the three modules.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours

Bibliography

1. A. Kalyan, I.K. Puri, “Advanced thermodynamics Engineering”, CRC Press, 2002.
2. P.W. Atkins, “Tratat de chimie fizică”, Ed. Tehnică, 1996.
3. I.G. Murgulescu, R. Valcu, “Introducere in chimia fizică. Termodinamica chimica”, vol III, Ed. Academiei RSR, Bucuresti, 1982.
4. I. Baldea, „Deducerea mecanismului de reacție”, Presa Universitară Clujeană, Cluj-Napoca, 2008.
5. I. Baldea, „Cinetica chimica si mecanisme de reactie. Baze teoretice si aplicatii”, Presa Universitara Clujeana, Cluj-Napoca, 2002.
6. G. Bozga, O. Muntean, „Reactoare chimice”, Vol. I + II, Editura Tehnică, Bucureşti, 2006.
7. O. Levenspiel, “Chemical Reactor Engineering”, Third Edition, John Wiley & Sons, 1999.

8. L. Oniciu, E. Constantinescu, „Electrochimie si coroziune", Editura Didactica si Pedagogica, Bucuresti, 1987. 9. L. Oniciu, L. Muresan, „Electrochimie aplicata", Presa Universitară Clujeană, Cluj-Napoca, 1998.		
8.2 Laboratory Practice	Teaching methods	Remarks
8.2.1. TD1: Calculation of thermodynamic quantities in open systems and irreversible systems.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.2. TD2: Case studies: phase diagrams for multi-component systems; interpretation of phase diagrams; azeotrope, eutectic, peritectic, chemical compound formation in solid phase.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.3. CK1: Determination of partial reaction orders and individual rate coefficients from diverse kinetic experimental data, by using adequate linearization or complex kinetic models. Interpretation of experimental rate laws from the point of view of reaction mechanism.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.4. CK2: Case studies – deduction and interpretation of rate laws for gas – solid and gas – liquid processes when various elementary steps (diffusion / reaction) are rate determining.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.5. CK3: Case studies – calculus of individual rate coefficients for various reaction schemes.		
8.2.6. EC1: Various calculations and applications to the chapters discussed within the lecture – part 1.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.7. EC1: Various calculations and applications to the chapters discussed within the lecture – part 2.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
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 mecansime de reactie. Baze teoretice si aplicatii", Presa Universitara Clujeana, Cluj-Napoca, 2002**.** 4. G. Niac, V. Voiculescu, I. Baldea, M. Preda, „Formule tabele probleme de chimie fizică", Editura Dacia, Cluj-Napoca, 1984. 5. 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	Written colloquia consisting of three sets of subjects corresponding to the TC,	100 %

	discussed during lectures; Correct use of learned concept within new contexts. Correct solving of problems as inherent part of examination subjects.	CC and EC modules of the course. Proven or intended fraud is punished according to the ECST rules of UBB.	(Each module contributes to the final mark with one third that is with 33.3 %)
10.5 Laboratory Practice	Correctness of answers – proper understanding and learning of concepts discussed during class; 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 exam, 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
March the 30th, 2017	Assoc. Prof. Dr. Eng. G. L. Turdean	Assoc. Prof. Dr. Eng. G. L. Turdean
	Prof. Dr. Liana Mureşan	Prof. Dr. Liana Mureşan
	Assoc. Prof. Dr. Eng. Alexandra. Csavdári	Assoc Prof. Dr. Eng. A. Csavdári

Date of approval	Signature of the head of department
March the 30th, 2017	Assoc. Prof. Dr. Eng. G. L. Turdean