

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 / Master's Degree

2. Information regarding the discipline

2.1 Name of the discipline	Advanced Physical Chemistry – CME6111						
2.2 Course coordinator	Prof. Dr. Maria Tomoaia-Cotișel (Thermodynamics „TC”) Prof. Dr. Liana Mureșan (Electrochemistry „EC”) Assoc. Prof. Dr. Eng. Alexandra Csavdări (Chemical Kinetics “CC”)						
2.3 Seminar coordinator	Lect.dr.Liviu-Dorel Bobo (Thermodynamics „TC”) Prof. Dr. Liana Mureșan (Electrochemistry „EC”) Assoc. Prof. Dr. Eng. Alexandra Csavdări (Chemical Kinetics “CC”)						
2.4. Year of study	I	2.5 Semester	1	2.6. Type of evaluation	C	2.7 Type of discipline	Mandatory

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					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	<ul style="list-style-type: none"> Not the case
4.2. competencies	<ul style="list-style-type: none"> Not the case

5. Conditions (if necessary)

5.1. for the course	<ul style="list-style-type: none">• The students will turn off their mobile phones• Delays will not be tolerated
5.2. for the seminar /lab activities	<ul style="list-style-type: none">• Students will attend the seminar with information of the course notes corresponding to the current seminar topic• Students will turn off their mobile phones• Delays will not be tolerated

6. Specific competencies acquired

Professional competencies	<ul style="list-style-type: none">• 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	<ul style="list-style-type: none">• 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	<ul style="list-style-type: none">• Approach of advanced concepts of physical chemistry (thermodynamics, chemical kinetics, electrochemistry).
7.2 Specific objective of the discipline	<ul style="list-style-type: none">• Advanced approach of the thermodynamics of open systems and of the heterogeneous equilibrium; Study of irreversible process and of statistical thermodynamics.• Interpretation of kinetic data from the point of view of rate laws and reaction mechanisms.• Approach of rate laws for heterogeneous 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. TC1: Thermodynamics of open systems.	Presentation; Explanation, Conversation; Description; Debate	

8.1.2. TC2: Heterogeneous equilibrium.	Presentation; Explanation, Conversation; Description; Debate	
8.1.3. TC3: concepts of irreversible process thermodynamics.	Presentation; Explanation, Conversation; Description; Debate	
8.1.4. TC4: Concepts and applications of statistic thermodynamics.	Presentation; Explanation, Conversation; Description; Debate	
8.1.5. CC1: Recap of fundamental concepts in chemical kinetics. Processing kinetic experimental data – general concepts, determination of reaction orders and rate coefficients.	Presentation; Explanation, Conversation; Description; Debate	
8.1.6. CC2: Interpretation of sub- and overunitary reaction orders from the point of view of reaction mechanisms.	Presentation; Explanation, Conversation; Description; Debate	
8.1.7. CC3: Rate laws and mechanisms for various types of heterogeneous uncatalysed processes (gas-solid and gas-liquid reactions)	Presentation; Explanation, Conversation; Description; Debate	
8.1.8. EC1: Recap of fundamental concepts in electrochemistry. The electric double layer.	Presentation; Explanation, Conversation; Description; Debate	
8.1.9. EC2: The Marcus Theory. Types of overpotential.	Presentation; Explanation, Conversation; Description; Debate	
8.1.10. EC3: Advanced electrochemical kinetics.	Presentation; Explanation, Conversation; Description; Debate	
8.1.11. EC4: Electrochemical investigation methods of electrode processes (classification, examples) and cyclic voltammetry.	Presentation; Explanation, Conversation; Description; Debate	
Bibliography 1. M. Tomoaia-Cotisel, I. Albu si E. Chifu, "Termodinamica Chimica", Presa Universitară Clujeană, Cluj-Napoca, 2009. 2. I. Haiduc, L. Bobos, „Chimia mediului si poluanti chimici”, Editura Fundatiei pentru Studii Europene, Cluj-Napoca, 2005. 3. I. Baldea, „Deducerea mecanismului de reacție”, Presa Universitară Clujeană, Cluj-Napoca, 2008. 4. G. Bozga, O. Muntean, „Reactoare chimice”, Vol. I + II, Editura Tehnică, București, 20016. 5. L. Oniciu, E. Constantinescu, „Electrochimie si coroziune”, Editura Didactica si Pedagogica, Bucuresti, 1987. 6. L. Oniciu, L. Muresan, „Electrochimie aplicata”, Presa Universitară Clujeană, Cluj-Napoca, 1998.		
8.2 Seminar	Teaching methods	Remarks
8.2.1. TC1: Modelling of chemical equilibrium	Explanation, Conversation; Description; Debate; Problem solving	
8.2.2. TC2: Case studies – phase diagrams for binary and ternary systems; interpretation of phase diagrams; azeotrope, eutectic, peritectic, chemical compound formation in solid phase.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.3. CC1: Determination of partial reaction orders and individual rate coefficients from diverse kinetic experimental data, by using adequate linearizations or complex kinetic models. Interpretation of experimental rate laws from the point of view of reaction mechanism.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.4. CC2: Case studies – deduction and nterpretation of rate laws for gas – solid and gas – liquid reactions	Explanation, Conversation; Description; Debate; Problem solving	

when various elementary steps (diffusion / reaction) are rate determining.		
8.2.5. EC1: Various calculations and applications to the chapters discussed within the lecture.	Explanation, Conversation; Description; Debate; Problem solving	
Bibliography 1. M. Tomoaia-Cotisel, O. Horovitz, A. Mocanu, I. Albu și Cs. Racz, “Termodinamica Chimica in Aplicații Numerice, Diagrame și Teste”, Editia a II-a, revăzută și adăugită, Presa Universitară Clujeană, 2008. 2. I. Baldea, „Cinetica Chimica si mecatisme de reactie. Baze teoretice si aplicatii”, Presa Universitara Clujeana, Cluj-Napoca, 2002. 3. G. Niac, V. Voiculescu, I. Baldea, M. Preda, „Formule tabele probleme de chimie fizică”, Editura Dacia Napoca, 1984.		

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	<p>Correctness of answers – proper understanding and learning of concepts discussed during lectures; Correct use of learned concept within new contexts.</p> <p>Correct solving of problems as inherent part of examination subjects.</p>	<p>Written colloquia consisting of three sets of subjects corresponding to the TC, CC and EC modules of the course.</p> <p>Proven or intended fraud is punished according to the ECST rules of UBB.</p>	<p>100 %</p> <p>(Each module contributes to the final mark with one third that is with 33.3 %)</p>
10.5 Seminar/lab activities	<p>Correctness of answers – proper understanding and learning of concepts discussed during seminars; Correct use of learned concept within new contexts.</p>	<p>Evaluated by means of problems to be solved, as inherent part of the examination subjects.</p>	-

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

30th of September 2012

Signature of course coordinator

Prof. Dr. Maria Tomoaia-Cotișel

Prof. Dr. Liana Mureșan

Assoc. Prof. Dr. Eng. Alexandra Csavdári

Signature of seminar coordinator

Lect.dr.Liviu-Dorel Boboș

Prof. Dr. Liana Mureșan

Assoc Prof. Dr. Eng. Alexandra Csavdári

Date of approval

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Signature of the head of department

Assoc. Prof. Dr. Eng. Mircea Cristea