

## 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	<b>Advanced Physical Chemistry – CME6111</b>						
2.2 Course coordinator	Assoc. Prof. Dr. Eng. Graziella Liana Turdean (Thermodynamics „TD”) Prof. Dr. Liana Muresan (Electrochemistry „EC”) Assoc. Prof. Dr. Eng. Alexandra Csavdári (Chemical Kinetics “CK”)						
2.3 Seminar coordinator	Assoc. Prof. Dr. Eng. Graziella Liana Turdean (Thermodynamics „TD”) Prof. Dr. Liana Muresan (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	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"> <li>• Not the case</li> </ul>
4.2. competencies	<ul style="list-style-type: none"> <li>• Not the case</li> </ul>

## 5. Conditions (if necessary)

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

## 6. Specific competencies acquired

<b>Professional competencies</b>	<ul style="list-style-type: none"> <li>• 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.</li> <li>• Use of advanced knowledge in the field of chemistry and chemical process engineering to explain and interpret chemical processes.</li> <li>• Identification and proper usage of concepts, method and theories for solving new complex problems of chemical process engineering.</li> <li>• Critical analysis and usage of principles, methods and advanced work techniques for quantitative and qualitative evaluation of chemical process engineering.</li> </ul>
<b>Transversal competencies</b>	<ul style="list-style-type: none"> <li>• Independent execution of complex professional duties and research projects using computer-aided techniques and comply with professional ethics and moral.</li> <li>• Planning, monitoring and assuming professional duties of underline group. Proving the coordination capabilities, analytical thinking, adaptability and flexibility, collaboration with team members.</li> <li>• Auto-evaluation of professional performances and establish the needs of continuous learning, documentation in the work fields in correlation with the labour market.</li> </ul>

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

7.1 General objective of the discipline	<ul style="list-style-type: none"> <li>• Approach of advanced concepts of physical chemistry (thermodynamics, chemical kinetics, electrochemistry).</li> </ul>
7.2 Specific objective of the discipline	<ul style="list-style-type: none"> <li>• Advanced approach in the field of thermodynamics of open systems and of irreversible processes; study of the thermodynamics of heterogeneous phase equilibrium</li> <li>• Correlation of advanced thermodynamics fundamentals and the ability to use / apply / correlate theoretical knowledge and interpret phenomena and processes associated in the field</li> <li>• Interpretation of kinetic data from the point of view of rate laws and reaction mechanisms.</li> <li>• Approach of rate laws for heterogeneous reaction systems.</li> <li>• 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</li> <li>• Training of students to use electrochemical investigation methods for the electrode processes; Cyclic voltammetry.</li> </ul>

## 8. Content

8.1 Course	Teaching methods	Remarks
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8.1.1. TD1: Review of the main concepts of chemical thermodynamics.	Presentation; Explanation, Conversation; Description; Debate	
8.1.2. TD2: Thermodynamics of open systems.	Presentation; Explanation, Conversation; Description; Debate	
8.1.3. TD3: Phase equilibrium in heterogeneous systems.	Presentation; Explanation, Conversation; Description; Debate	
8.1.4. TD4: Thermodynamics of irreversible process.	Presentation; Explanation, Conversation; Description; Debate	
8.1.5. CK1: Recap of fundamental concepts in chemical kinetics. Processing kinetic experimental data – general concepts, determination of reaction orders and rate coefficients. Empirical rate laws.	Presentation; Explanation, Conversation; Description; Debate	
8.1.6. CK2: Interpretation of rate laws (of reaction orders) from the point of view of reaction mechanisms.	Presentation; Explanation, Conversation; Description; Debate	
8.1.7. CK3: Rate laws and mechanism types in heterogeneous catalysis.	Presentation; Explanation, Conversation; Description; Debate	
8.1.8. CK4: Rate laws and mechanism types for heterogeneous un-catalysed processes.	Presentation; Explanation, Conversation; Description; Debate	
8.1.9. EC1: Recap of fundamental concepts in electrochemistry. The electric double layer.	Presentation; Explanation, Conversation; Description; Debate	
8.1.10. EC2: The Marcus Theory. Types of overpotential.	Presentation; Explanation, Conversation; Description; Debate	
8.1.11. EC3: Advanced electrochemical kinetics.	Presentation; Explanation, Conversation; Description; Debate	
8.1.12. EC4: Electrochemical investigation methods of electrode processes (classification, examples) and cyclic voltammetry.	Presentation; Explanation, Conversation; Description; Debate	
<b>Bibliography</b>		
<ol style="list-style-type: none"> <li>1. A. Kavian, Ed. Pinar, "Advanced thermodynamics Engineering", CRC Press, 2002.</li> <li>2. P. V. Arora, "Termodinamica fizica", Ed. Tehnica, 1996.</li> <li>3. I. C. Mărgulescu, E. Văduva, "Tratat de chimia fizica, Termodinamica chimica", vol III, Ed. Academiei R.S.R., Bucuresti, 1972.</li> <li>4. I. Baldea, "Determinarea energiei de reactie", Presa Universitara Clujeana, Cluj-Napoca, 2008.</li> <li>5. I. Baldea, „Cinetica chimica si mecanisme de reactie. Baze teoretice si aplicatii”, Presa Universitara Clujeana, Cluj-Napoca, 2002.</li> <li>6. G. Bozga, O. Muntean, „Reactoare chimice”, Vol. I + II, Editura Tehnica, Bucuresti, 2006.</li> <li>7. L. Oniciu, E. Constantinescu, „Electrochimie si coroziune”, Editura Didactica si Pedagogica, Bucuresti, 1987.</li> <li>8. L. Oniciu, L. Muresan, „Electrochimie aplicata”, Presa Universitara Clujeana, Cluj-Napoca, 1998.</li> </ol>		
<b>8.2 Seminar</b>	<b>Teaching methods</b>	<b>Remarks</b>
8.2.1. TD1: Calculation of thermodynamic quantities in open systems and irreversible systems.	Explanation, Conversation; Description; Debate; Problem solving	
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	
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	Explanation, Conversation; Description; Debate; Problem solving	

mechanism.		
8.2.4. CK2: Case studies – deduction and interpretation of rate laws for: heterogeneously catalysed reactions (expressing superficial concentrations from adsorption isotherms); gas – solid and gas – liquid reactions when various elementary steps (diffusion / reaction) are rate determining.	Explanation, Conversation; Description; Debate; Problem solving	
8.2.5. EC1: Various calculations and applications to the chapters discussed within the lecture.	Explanation, Conversation; Description; Debate; Problem solving	
<b>Bibliography</b>		
<ol style="list-style-type: none"> <li>1. P.W. Atkins, J. De Paula, "Chimie Fizica", Ed. AGIR, 2003.</li> <li>2. H. E. Avery, D. J. Shaw, "Basic Physical Chemistry Calculations", Butterworth &amp; Co., 1980.</li> <li>3. I. Baldea, „Cinetica Chimica si mecanisme de reactie. Baze teoretice si aplicatii”, Presa Universitara Clujeana, Cluj-Napoca, 2002.</li> <li>4. G. Niac, V. Voiculescu, I. Baldea, M. Preda, „Formule tabele probleme de chimie fizica”, Editura Dacia, Cluj-Napoca, 1984.</li> <li>5. Notes provided by lecturers.</li> </ol>		

### 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 steted 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 % (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

Signature of course coordinator

Signature of seminar coordinator

October 30, 2013

Assoc. Prof. Dr. Eng. G. L. Turdean

Assoc. Prof. Dr. Eng. G. L. Turdean

Prof. Dr. Liana Muresan

Prof. Dr. Liana Muresan

Assoc. Prof. Dr. Eng. Alexandra. Csavdári

Assoc Prof. Dr. Eng. Al. Csavdári

Date of approval

Signature of the head of department

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Assoc. Prof. Dr. Eng. Mircea Cristea

