UNIVERSITATEA BABEŞ-BOLYAI
BABEŞ-BOLYAI TUDOMÁNYEGYETEM
BABEŞ-BOLYAI UNIVERSITÄT
BABEŞ-BOLYAI UNIVERSITY
TRADITIO ET EXCELLENTIA

Tradiție și Excelență prin
Cultură - Știință - Inovație din 1581

Facultatea de Chimie și Inginerie Chimică
Str. Arany János nr. 11
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SYLLABUS

Advanced Pysical Chemistry

University year 2025-2026

1. Information regarding the programme

1.1. Higher education institution	Babeş-Bolyai University
1.2. Faculty	Faculty of Chemistry and Chemical Engineering
1.3. Department	Department of Chemical Engineering
1.4. Field of study	Chemical Engineering
1.5. Study cycle	Master
1.6. Study programme/Qualification	Advanced Process Chemical Engineering
1.7. Form of education	Full-time education

2. Information regarding the discipline

2.1. Name of the discipline	**Advanced Pysical Chemistry**					Discipline code	**CME6111**
2.2. Course coordinator	Assoc. Prof. dr. eng. Adrian Nicoară (Thermodynamics „TD" and Electrochemistry) Assoc. Prof. dr. eng. Alexandra Ana Csavdari (Chemical Kinetics "CK")						
2.3. Seminar coordinator	Assoc. Prof. dr. eng. Adrian Nicoară (Thermodynamics „TD" and Electrochemistry) Assoc. Prof. dr. eng. Alexandra Ana Csavdari (Chemical Kinetics "CK")						
2.4. Year of study	I	2.5. Semester	1	2.6. Type of evaluation	E	2.7. Discipline regime	DF/Compulsory

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

3.1. Hours per week	**4**	of which: 3.2 course	**2**	3.3 seminar/laboratory	**2/0**
3.4. Total hours in the curriculum	56	of which: 3.5 course	28	3.6 seminar/laborator	**28/0**
Time allotment for individual study (ID) and self-study activities (SA)					**hours**
Learning using manual, course support, bibliography, course notes (SA)					14
Additional documentation (in libraries, on electronic platforms, field documentation)					14
Preparation for seminars/labs, homework, papers, portfolios and essays					28
Tutorship					7
Evaluations					6
Other activities:					
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	• Students will punctually join the class.

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	• Students will follow the sanitary regulations in place. • Rules of good practice will be explained by the lecturer at the beginning of the semester and will be followed accordingly by all participants to the class. • During class, students will keep their mobile phones and any other gadgets on silent mode and out of sight.
5.2. for the seminar /lab activities	• Students will punctually join the class (either *on-site* or *on-line*). • If *on-site*: Students will follow the sanitary regulations in place. • Students will bring adequate writing and computing devices (laptops). • Rules of good practice will be explained by the lecturer at the beginning of the semester and will be followed accordingly by all participants to the class. • During class, students will keep their mobile phones and any other gadgets on silent mode and out of sight.

6. Specific competencies acquired [1]

Professional/essential 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).

[1] One can choose either competences or learning outcomes, or both. If only one option is chosen, the row related to the other option will be deleted, and the kept one will be numbered 6.

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7.2 Specific objective of the discipline	• Advanced approach in the field of thermodynamics of reversible and of irreversible processes. • Correlation of advanced thermodynamics fundamentals and the ability to use / apply / correlate theoretical knowledge and interpret phenomena and processes associated in the field. • 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). • Training of students to use electrochemical investigation methods for the electrode processes; Cyclic voltammetry. • Interpretation of kinetic data from the point of view of rate laws and reaction mechanisms. • Interpretation of kinetic data for complex reaction systems in homogeneous and heterogeneous media.

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	Alocated time = 2 hours
8.1.2. TD2: Introduction in irreversible processes thermodynamics. Basic concepts. Local equilibrium hypostesis. Entropy balance.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.3. TD3: General theory of irreversible process thermodynamics: 7 steps formulation.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.4. TD4: Minimum entropy production principle. Application to heat transport.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.5. TD5: Irreversible thermodynamics of electrokinetic phenomena and membrane processes.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.6. EC1: Recap of fundamental concepts in electrochemistry. The electric double layer. Double layer and electrokinetic phenomena.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.7. EC2: Advanced electrochemical kinetics.Types of overpotential. Electrode kinetic law for multielectrone transfer processes.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.8. EC3: Horiuti number. Mass transport overpotential.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.9. EC4: Electrochemical investigation methods of electrode processes (classification, examples) and cyclic voltammetry.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.10. 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
8.1.11. CK2: Methods of obtaining experimental data Processing kinetic experimental data – general concepts,	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours

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determination of reaction orders and rate coefficients. Empirical rate laws.		
8.1.12. CK3: Empirical rate laws – continuation. Interpretation of rate laws from the point of view of reaction mechanisms.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.13. CK4: Determination of individual rate coefficient for some complex reaction systems in homogeneous and heterogeneous media – Part 1.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
8.1.14. CK5: Determination of individual rate coefficient for some complex reaction systems in homogeneous and heterogeneous media – Part 2.	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, "*Physical Chemistry*", any edition.
3. I.G. Murgulescu, R. Valcu, "*Introducere in chimia fizică. Termodinamica chimică*", vol III, Ed. Academiei RSR, Bucuresti, 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, 2000.
7. G. Bozga, O. Muntean, „*Reactoare chimice*", Vol. I + II, Editura Tehnică, Bucureşti, 2006.
8. O. Levenspiel, "*Chemical Reactor Engineering*", Third Edition, John Wiley & Sons, 1999.
9. L. Oniciu, E. Constantinescu, „*Electrochimie Si coroziune*", Editura Didactică şi Pedagogică, Bucureşti, 1987.
10. L. Oniciu, L. Mureşan, „*Electrochimie aplicată*", Presa Universitară Clujeană, Cluj-Napoca, 1998.
11. PPT presentations – available in revised form during the semester.

8.2 Seminar	Teaching methods	Remarks
8.2.1. TD1: Applications to first law of thermodynamics.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.2. TD2: Applications to second law of thermodynamics.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.3. TD3: Applications to general irreversible thermodynamics.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.3. TD4: Numerical applications of irreversible processes thermodynamics: heat transfer examples.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.4. TD5: Numerical applications of irreversible processes thermodynamics: membrane processes examples.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.6. EC1: Double layer numerical examples.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.7. EC2: Electrode kinetics applications: activation control.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.8. EC3: Electrode kinetics applications: mass transport control.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours

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8.2.9. EC4: Investigation methods.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.10. 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 – part I.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.11. CK2: 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 – part II.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.12. CK3: Case studies – calculus of individual rate coefficients for various reaction schemes in homogeneous and heterogeneous media – part 1.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.13. CK4: Case studies – calculus of individual rate coefficients for various reaction schemes in homogeneous and heterogeneous media – part 2.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours
8.2.14. Case studies from the chemical industry.	Explanation, Conversation; Description; Debate; Problem solving	Alocated time = 2 hours

Bibliography

1. P.W. Atkins, P.W. Atkins, "*Physical Chemistry*", any edition.
2. H. E. Avery, D. J. Shaw, "*Basic Physical Chemistry Calculations*", Butterworth & Co., 1980.
3. I. Bâldea, „*Cinetică chimică și mecanisme de reacție. Baze teoretice și aplicații*", Presa Universitară Clujeană, Cluj-Napoca, 2002.
4. I. Bâldea, „*Some advanced topics in chemical kinetics*", Cluj University Press, 2000.
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 – available during the semester.

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 acquire a consistent body of knowledge, in accordance with the skills of the Diploma Supplement and the qualifications of the ANC.

10. Evaluation

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Percentage of final grade
10.4 Course	Correctness of answers – proper understanding and learning of concepts	Written exam consisting of three sets of subjects, theory and exercises,	100 %

	discussed during lectures; Correct use of learned concept within new contexts. Correct solving of problems as inherent part of examination subjects.	corresponding to the TC, CK and EC, respectively. 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 Seminar/laboratory	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. Teachers may ask students to solve homework during the semester, as part of their formative evaluation.	-
10.6 Minimum standard of performance			
• Grade 5 (five) at the written exam, at **each** of the three separate modules of the course (TD, EC and CK). The final mark represents the rounded value of the average of the marks obtained at each of the three modules. • Adequate knowledge and usage of basic concepts of advanced physical chemistry.			

11. Labels ODD (Sustainable Development Goals)[2]

	Quality Education

Date:
14.04.2025

Signature of course coordinator

Assoc. Prof. dr. eng. Adrian Nicoară

Signature of seminar coordinator

Assoc. Prof. dr. eng. Adrian Nicoară

Assoc. Prof. dr. eng. Alexandra Ana Csavdari

Assoc. Prof. dr. eng. Alexandra Ana Csavdari

Date of approval:
15.04.2025

Signature of the head of department

Prof. Habil. Dr. Eng. Graziella Liana Turdean

[2] Keep only the labels that, according to the *Procedure for applying ODD labels in the academic process*, suit the discipline and delete the others, including the general one for *Sustainable Development* – if not applicable. If no label describes the discipline, delete them all and write „*Not applicable*.".