COURSE DESCRIPTION

Advanced Pysical Chemistry

Academic year 2026 - 2027

1. Programme-related data

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	Chemical Engineering
1.5. Level of study	Master
1.6. Degree programme / Qualification	Advanced Process Chemical Engineering
1.7. Form of education	Full-time education

2. Course-related data

2.1. Course title	**Advanced Physical Chemistry**			Course 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	1	2.5. Semester	1	2.6. Type of assessment	Exam
2.7. Course status	Compulsory			2.8. Course type	Core subject

3. Total estimated time (hours per semester of teaching activities)

5	**4**	of which: 3.2. course	**2**	3.3. seminar/ laboratory/ project	**2**
3.4. Total of hours in the curriculum	56	of which: 3.5. course	28	3.6. seminar/ laboratory	**28**
Time allocation for individual study (IS) and self-taught activities (ST)					**hours**
Learning from textbooks, course materials, bibliography, and notes (IS)					14
Additional research in the library, on subject-specific electronic platforms, and on-site					14
Preparing seminars/ laboratories/ projects, assignments, reports, portfolios, and essays					28
Tutoring (professional guidance)					7
Examinations					6
Other activities					-
3.7. Total hours of individual study (IS) and self-taught activities (ST)				**69**	
3.8. Total hours per semester				**125**	
3.9. Number of credits				**5**	

4. Prerequisites (where applicable)

4.1. curriculum-related	Not the case
4.2 skills-related	Not the case

5. Specific conditions (where applicable)

5.1. course-related	• Students will punctually join the class and 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. seminar/laboratory-related	• Students will punctually join the class and follow the sanitary regulations in place. • Students will bring adequate writing and computing devices. • 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.

6.1. Competencies resulting from the completion of the degree programme *(as referred to in the curriculum)*[1]

Professional competencies	
Competency code	**Competency**
PC1	Description, analysis and use of elaborate theories and concepts in the fields of chemistry and process advanced chemical engineering.
PC3	Development and use of mathematical models and simulators in process engineering for diagnosis of problems, analysis of optimum operating systems and control of (bio)chemical processes.
Transversal competencies	
Competency code	**Competency**
TC1	Independent execution of complex professional assignments and autonomous development of project-research activities by using computer-assisted techniques and by observing the norms of professional ethics and moral conduct.

6.2. Learning outcomes relevant to the degree programme (as referred to in the curriculum)[2]

Learning outcomes targeted by the subject		
Competency code	**Knowledge and comprehension**	**Specific academic skills**
PC1 **PC4** **TC1**	1. Formulation of solutions to solve complex chemical engineering problems based on knowledge, identification and application of advanced concepts, methods, and theories in the field of chemical engineering and chemistry.	1. Critical analysis and application of advanced principles, methods, and techniques for the evaluation, design, and development of new products and technologies.
PC1 **PC3** **TC1**	2. Explain and understand the operation of devices, equipment and processes in the chemical process industries based on software environments that describe their behaviour using complex analytical or statistical mathematical models	2. Use of mathematical models for technological design and their implementation in automatic control systems, in order to obtain optimal solutions for economically and energetically operation, associated to low environmental impact.

7. Subject-specific learning outcomes

Knowledge and comprehension
1. The student/graduate understands (defines and explains) advanced concepts of chemistry-physics (thermodynamics, chemical kinetics, and electrochemistry) with application in chemical engineering.
2. The student/graduate understands (defines and explains) scientific investigation strategies that elucidate the physicochemical aspects of processes with application in chemical engineering.

[1] The professional and/or transversal skills targeted by the subject for which the course description is prepared will be copied from the curriculum of the degree programme. For each competency, the complete entry, including the competency code, will be copied with the exact wording that appears in the curriculum, without any changes. If no competency is copied from either of the two categories, the row corresponding to that category is deleted from the table.

[2] The learning outcomes relevant for the degree programme and targeted by the subject for which the course description is prepared will be listed. The entries, copied without any changes from the Curriculum by subject type (Core Subject/Specialisation Subject/Complementary Subject), are listed under the corresponding competency.

Specific academic skills
1. The student/graduate applies advanced concepts of chemistry-physics (thermodynamics, chemical kinetics, and electrochemistry) with significance in chemical engineering.
2. The student/graduate applies scientific investigation strategies to obtain specific data from industrial installations, processes and interprets the data obtained.
3. The student/graduate elucidates the physicochemical aspects of processes with application in chemical engineering.

8. Contents

8.1. Course	**Teaching and learning methods**	**Remarks[3]**
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, determination of reaction orders and rate coefficients. Empirical rate laws.	Presentation; Explanation, Conversation; Description; Debate	Alocated time = 2 hours
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

[3] For example, organisational aspects, recommendations for students, specific aspects relating to the course/seminar, such as inviting experts in the field, etc.

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 and learning 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
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 şi mecanisme de reacţie. Baze teoretice şi aplicaţii*", 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. Evaluation

Type of activity	9.1 Evaluation criteria[4]	9.2 Evaluation methods[5]	9.3 Percentage in the final grade
9.4. 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 exam consisting of three sets of subjects, theory and exercises, corresponding to the TC, CK and EC, respectively. 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 %)
9.5. 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.	-

9.6 Minimum standard for passing

- 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.

[4] The evaluation criteria must directly reflect the learning outcomes targeted at the level of the degree programme respectively at the level of the subject. More specifically, the learning outcomes set out in the expected learning outcomes are assessed.

[5] Both final evaluation methods and ongoing evaluation strategies should be established.

10. SDG labels (Sustainable Development Goals)[6]

	○	Sustainable Development Generic Label

								
○	○	○	◉	○	○	○	○	○
								No label applies
○	○	○	○	○	○	○	○	○

Date of entry:
4.05.2026

Signature of course coordinator

Assoc. Prof. dr. eng. Adrian Nicoară

Assoc. Prof. dr. eng. Alexandra Ana Csavdari

Signature of seminar coordinator

Assoc. Prof. dr. eng. Adrian Nicoară

Assoc. Prof. dr. eng. Alexandra Ana Csavdari

Date of approval in the department:
4 mai 2026

Signature of the head of department

Prof. Habil. Dr. Eng. Graziella Liana Turdean

[6] Select a single label which, according to the *Implementation of SDG labels in the academic process*, best matches the subject. If the subject addresses sustainable development in a generic manner (i.e. by presenting/introducing the general framework of sustainable development, etc.), then the Sustainable Development generic label may be applied. If none of the labels describe the subject, select the last option: *"No label applies."*