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. Adrian Nicoară (Thermodynamics „TD" and Electrochemistry) Assoc. Prof. Dr. Eng. Alexandra Csavdári (Chemical Kinetics "CK")						
2.3 Seminar / laboratory work coordinator	Assoc. Prof. dr. eng. Adrian Nicoară (Thermodynamics „TD" and Electrochemistry) 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	DF/Comp

DF=Fundamental discipline

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

3.1 Hours per week	2	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/laboratory	28/0
Time allotment:					hours
Learning using manual, course support, bibliography, course notes					31
Additional documentation (in libraries, on electronic platforms, field documentation)					7
Preparation for seminars/labs, homework, papers, portfolios and essays					14
Tutorship					14
Evaluations					3
Other activities: not the case					-

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 enter the class (lecture hall or *on-line* platform) with turned-off or silent mode mobile phones / gadgets. These will be kept out of sight.

	• In *on-line* environment, the students will have functioning and open camera, functioning but turned off microphones (as long as other people) speak. • Delays will not be tolerated.
5.2. for the seminar /lab activities	• Students will bring to the seminar their course notes and appropriate calculus device (laptops). • Students will enter the class (seminar hall or *on-line* platform) with turned-off or silent mode mobile phones / gadgets. These will be kept out of sight. • In *on-line* environment, the students will have functioning and open camera, functioning but turned off microphones (as long as other people) speak. • 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 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, 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
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
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	Explanation, Conversation; Description; Debate;	Alocated time = 2 hours

and heterogeneous media – part 2.	Problem solving	
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. 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 assimilating the theoretical and methodological concepts and by approaching the practical aspects included in the **Advanced Physical Chemistry** discipline, the students acquire consistent knowledge in accordance with the competences of the Diploma Supplement and qualifications in the ANC

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 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. <u>Note</u>*: The exact details of examination depend on the epidemiologic context.* 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 %)
10.5 Seminar / 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. Teachers may ask students to solve homework during the semester, as part of their formative evaluation.	-

10.6 Minimum performance standards
• 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.

Date	Signature of course coordinator	Signature of seminar coordinator
April the 10th, 2024	Assoc. Prof. Dr. Eng. Adrian Nicoară	Assoc. Prof. Dr. Eng. Adrian Nicoară
	Assoc. Prof. Dr. Eng. Alexandra Csavdári	Assoc Prof. Dr. Eng. A. Csavdári

Date of approval	Signature of the head of department
22.04.2024	Prof. Dr. Eng. Graziella Liana Turdean