**SYLLABUS**

**1. Information regarding the programme**

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| 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**

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|---|---|---|---|---|---|---|---|
| 2.1 Name of the discipline | **Advanced Physical Chemistry – CME6111** | | | | | | |
| 2.2 Course coordinator | Assoc. Prof. dr. eng. Adrian Nicoară (Thermodynamics „TD" and Electrochemistry)<br>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)<br>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 | Ob |

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

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|---|---|---|---|---|---|
| 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 | | | | | - |

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| 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)

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| 4.1. curriculum | • Not the case |
| 4.2. competencies | • Not the case |

**5. Conditions** (if necessary)

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|---|---|
| 5.1. for the course | • The students will turn off their mobile phones or put them on silent mode<br>• Delays will not be tolerated |
| 5.2. for the seminar /lab activities | • Students will bring to the laboratory practice their course notes and appropriate calculus device<br>• Students will turn off their mobile phones or put them on silent mode<br>• Delays will not be tolerated |

**6. Specific competencies acquired**

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| **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.<br>• Use of advanced knowledge in the field of chemistry and chemical process engineering to explain and interpret chemical processes.<br>• Identification and proper usage of concepts, method and theories for solving new complex problems of chemical process engineering.<br>• 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.<br>• Planning, monitoring and assuming professional duties of underline group. Proving the coordination capabilities, analytical thinking, adaptability and flexibility, collaboration with team members.<br>• 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)

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| 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.<br>• Correlation of advanced thermodynamics fundamentals and the ability to use / apply / correlate theoretical knowledge and interpret phenomena and processes associated in the field.<br>• 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).<br>• Training of students to use electrochemical investigation methods for the electrode processes; Cyclic voltammetry.<br>• Interpretation of kinetic data from the point of view of rate laws and reaction mechanisms.<br>• 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 media. | Presentation; Explanation, Conversation; Description; Debate | Alocated time = 2 hours |
| 8.1.14. CK5: Determination of individual rate coefficient for some complex reaction systems in heterogeneous media. | 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 chimica", vol III, Ed. Academiei RSR, Bucuresti, 1982.
4. I. Baldea, „Deducerea mecanismului de reacţie", Presa Universitară Clujeană, Cluj-Napoca, 2008.
5. I. Baldea, „Cinetica chimica si mecanisme de reactie. Baze teoretice si aplicatii", Presa Universitara Clujeana, Cluj-Napoca, 2002.

6. I. Baldea, „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 Didactica si Pedagogica, Bucuresti, 1987.
10. L. Oniciu, L. Muresan, „Electrochimie aplicata”, 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 media. | 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 heterogeneous media. | Explanation, Conversation; Description; Debate; Problem solving | Alocated time = 2 hours |
| 8.2.14. Recap and preparation for the exam. | 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. Baldea, „Cinetica Chimica si mecansime de reactie. Baze teoretice si aplicatii", Presa Universitara Clujeana, Cluj-Napoca, 2002**.**
4. I. Baldea, „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 will get the knowledge in accordance with the competencies of the Diploma Supplement and the qualifications of 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. | Written colloquia consisting of three sets of subjects corresponding to the TC, CC and EC modules of the course.<br><br>Proven or intended fraud is punished according to the ECST rules of UBB. | 100 %<br><br>(Each module contributes to the final mark with one third that is with 33.3 %) |
| | Correct solving of problems as inherent part of examination subjects. | | |
| 10.5 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. | - |

| 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.<br>• Adequate knowledge and usage of basic concepts of advanced physical chemistry. |

| Date | Signature of course coordinator | Signature of seminar coordinator |
| --- | --- | --- |
| April the 15th, 2020 | 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 |
| --- | --- |
| April the 16th, 2020 | Prof. Dr. Eng. G. L. Turdean |