SYLLABUS
Spring semester 2020-2021 academic years
on the educational program "7M07103 Chemical Engineering "

Discipline's code	Discipline's title	Independent work of students (IWS)	No. of hours per week			Number of credits	Independent work of student with teacher (IWST)
			Lectures (L)	Practical training (PT)	Laboratory (Lab)		
ME 5305	Modelling in electrochemistry	12	15	30	-	5	7

Academic course information					
Form of education	**Type of course**	**Types of lectures**	**Types of practical training**	**Number of IWS**	**Form of final control**
Offline/ traditional	practical	Traditional, oral presentation	Problems, creating a simulation model of electrochemical processes by using COMSOL Multiphysics software	12	Traditional/ in the platform Oqylyq
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Academic presentation of the course

Aim of course	Expected Learning Outcomes (LO) As a result of studying the discipline the undergraduate will be able to:	Indicators of LO achievement (ID) (for each LO at least 2 indicators)
This course will introduce the key principles and techniques used to model electrochemical. Each case will start with the physical and chemical aspects of the model then move on to the numerical approach appropriate for the problem. The module will consider dedicated electrochemistry modelling software COMSOL Multiphysics.	1. Explain the principles of modelling electrochemical systems. Appraise the use of modelling in electrochemical research	1.1. Use electrochemical modelling terminology and concepts 1.2. Explain the principles of charge transfer and mass transfer stages of electrode reaction 1.3. Structure and properties of electrical double layer, charge transfer through double layer
	2. Select a computational or numerical technique appropriate for a given electrochemical process	2.1. Principles of electrochemical methods. Chronoamperometry. 2.2. Application and theory of voltammetry. 2.3. Investigation of electrochemical behaviour of electrode/electrolyte interface using cyclic voltammetry method
	3. Explain the principles of key computational and numerical modelling techniques used in electrochemical science	3.1. Modelling of electrochemical impedance spectroscopy measurements of simple electrochemical systems 3.2. Explain fundamentals of electrodeposition 3.3. Modelling of decorative electroplating in COMSOL Multiphysics
	4. Assess the limitations of these key methods simulate basic electrochemical processes	4.1. Modelling of common electrochemical reactors 4.2. Modelling of copper electrodeposition in Rotating Cylinder Hull Cell type reactor 4.2. Asses the opportunities of lead-acid battery modelling in COMSOL Multiphysics
	5. Use available electrochemical modelling software to simulate complex electrochemical processes	5.1. Modelling of chemical power sources using COMSOL Multiphysics 5.2. Rechargeable secondary power sources, modelling by COMSOL Multiphysics 5.3. Lithium-ion battery, modelling by COMSOL Multiphysics

Prerequisites	**Mathematics 2, Chemical Kinetics and Electrochemistry, Modeling of Chemical-Technological Processes, Theoretical electrochemistry.**
Post requisites	**Macrokinetics of chemical processes and reactor design**
Information resources	**References:** 1. Bard A. J. et al. Electrochemical methods: fundamentals and applications. – New York : wiley, 1980. – T. 2. 2. Sanecki P. T., Skitał P. M. Mathematical Modeling of Electrode Processes–Potential Dependent Transfer Coefficient in Electrochemical Kinetics //Recent Trend in Electrochemical Science and Technology. – IntechOpen, 2012. 3. Franco A. A., Doublet M. L., Bessler W. G. (ed.). Physical multiscale modeling and numerical simulation of electrochemical devices for energy conversion and storage: from theory to engineering to practice. – Springer, 2015. 4. Gabrielli C., Perrot H. Modeling and Numerical Simulations II //In Modern Aspects of Electrochemistry, Springer, New York. – 2009. – C. 151-238. 5. Franco A. A., Doublet M. L., Bessler W. G. (ed.). Physical multiscale modeling and numerical simulation of electrochemical devices for energy conversion and storage: from theory to engineering to practice. – Springer, 2015. ***Articles:*** 6. Gu W. B., Wang C. Y., Liaw B. Y. Numerical modeling of coupled electrochemical and transport processes in lead□acid batteries //Journal of The Electrochemical Society. – 1997. – T. 144. – №. 6. – C. 2053-2061. 7. Paz-García J. M. et al. Modeling of electrokinetic processes by finite element integration of the Nernst–Planck–Poisson system of equations //Separation and Purification Technology. – 2011. – T. 79. – №. 2. – C. 183-192. 8. Vakhrushev A., Molchanov E. Hydrodynamic Modeling of Electrocodeposition on a Rotating Cylinder Electrode //Key Engineering Materials. – Trans Tech Publications, 2015. – T. 654. – C. 29-33. 9. Avchukir K., Burkitbayeva B. D. Conductive Polymer/SiO2 Composite as an Anticorrosive Coating Against Carbon Dioxide Corrosion of Mild Steel. A Simulation Study //Eurasian Chemico-Technological Journal. – 2020. – T. 22. – №. 4. – C. 295-303.
Academic policy of the course in the context of university moral and ethical values	**Academic Behavior Rules:** All students have to register at the MOOC. The deadlines for completing the modules of the online course must be strictly observed in accordance with the discipline study schedule. ATTENTION! Non-compliance with deadlines leads to loss of points! The deadline of each task is indicated in the calendar (schedule) of implementation of the content of the curriculum, as well as in the MOOC. **Academic values:** - Practical trainings/laboratories, IWS should be independent, creative. - Plagiarism, forgery, cheating at all stages of control are unacceptable. - Students with disabilities can receive counseling at e-mail *******@gmail.com.
Evaluation and attestation policy	**Criteria-based evaluation:** assessment of learning outcomes in relation to descriptors (verification of the formation of competencies in midterm control and exams). **Summative evaluation:** assessment of work activity in an audience (at a webinar); assessment of the completed task.

CALENDAR (SCHEDULE) THE IMPLEMENTATION OF THE COURSE CONTENT:

weeks	Topic name	LO	ID	amount of hours	Maximum score	Form of Knowledge Assessment	The Form of the lesson / platform
Module 1							
1	**L.1** Introduction to the modelling of electrochemical processes	LO 1	ID 1.1.	1			Offline/traditional
1	**PT 1** Benefits of using COMSOL Multiphysics in modelling of electrochemical reactors	LO 1	ID 1.1.	2	10	TK and/or IT	
1	IWSP 1 Consultation on the implementation of IWS1	LO 1	ID 1.1.	1			

2	**L.2** Basic concepts of electrochemical processes, the stages of electrode reaction.	LO 1	ID 1.2.	1			Offline/traditional
2	**PT 2** Modelling of diffuse double layer	LO 1	ID 1.2.	2	15	TK and/or IT	
2	**IWS 1.** Course in Coursera: *Simulation and modeling of natural processes.* Assignment 1. https://www.coursera.org/learn/modeling-simulation-natural-processes#syllabus	LO 1	ID 1.2.		10	IT	
3	**L.3** Electrical double layer (DL). Charge transfer through DL	LO 1	ID 1.3.	1			Offline/traditional
3	**PT 3** Modelling of diffuse DL with charge transfer	LO 1	ID 1.3.	2	10	TK and/or IT	
3	IWSP 2 Consultation on the implementation of IWS2	LO 1	ID 1.3.	1	5	CW, QS	
3	**IWS 2.** Course in Coursera: *Simulation and modeling of natural processes.* Assignment 2. https://www.coursera.org/learn/modeling-simulation-natural-processes#syllabus	LO 1	ID 1.3.		5	IT	
4	**L.4** Electrochemical methods. Chrono-amperometry. Mass transfer kinetics.	LO 2	ID 2.1.	1			Offline/traditional
4	**PT 4** One dimensional modelling of thin layer chronoamperometry in COMSOL Multiphysics	LO 2	ID 2.1.	1	10	TK and/or IT	
4	**IWS 3.** Course in Coursera: *Simulation and modeling of natural processes.* Assignment 3-4. https://www.coursera.org/learn/modeling-simulation-natural-processes#syllabus	LO 2	ID 2.1.		8	IT	
5	**L.5** Techniques based on microelectrodes. Voltammetry of a microdisk electrode.	LO 2	ID 2.2.	1			Offline/traditional
5	**PT 5** 2D axisymmetric modelling of voltammetry at a microdisk electrode	LO 2	ID 2.2.	2	10	TK and/or IT	
5	IWSP 4 Consultation on the implementation of IWS4	LO 2	ID 2.2.	1	2	CW, QS	
5	**IWS 4** Course in Coursera: *Simulation and modeling of natural processes.* Assignment 5-7. https://www.coursera.org/learn/modeling-simulation-natural-processes#syllabus	LO 2	ID 2.2.		8	IT	
5	**MT 1**	LO 1 - LO 2	ID 1.1. - ID 2.2.		100		
6	**L.6** Analytical techniques for investigating electrochemical reactions. Cyclic voltammetry.	LO 2	ID 2.3.	1			Offline/traditional
6	**PT 6** Creating simulation model of cyclic voltammetry of simple one electron reaction in COMSOL Multiphysics	LO 2	ID 2.3.	1	10	TK and/or IT	
6	**IWS 5** Course in Coursera: *Simulation and modeling of natural processes.* Practice exercise. https://www.coursera.org/learn/modeling-simulation-natural-processes#syllabus	LO 2	ID 2.3.		8	IT	
7	**L.1** Techniques based on concepts of impedance	LO 3	ID 1.1.	1			Offline/traditional
7	**PT 1** Electrochemical impedance spectroscopy	LO 3	ID 5.1.	2	10	TK and/or IT	
7	IWSP 6 Consultation on the implementation of IWS6	LO 3	ID 3.1.	1		CW, QS	
7	**IWS 6** Course in Coursera: *Simulation and modeling of natural processes.* Summarising. Preparing oral presentation.	LO 3	ID 3.1.		10	IT	

Module II							
8	**L.8** Electrochemical deposition of metals. Reaction mechanism and the basic stages.	LO 3	ID 3.2	1			
8	**PT 8** Drawing of 3D geometry of the electrode for modelling of electrochemical plating of nickel	LO 3	ID 3.2	2	15	TK and/or IT	
9	**L.9** Modelling of the metal finishing technologies. Electroplating. Reaction kinetics.	LO 3	ID 3.3.	1			Offline/traditional
9	**PT 9** Modelling of nickel plating in COMSOL Multiphysics.	LO 3	ID 3.3.	2	15	TK and/or IT	
9	IWSP 7 Consultation on the implementation of IWS7	LO 3	ID 3.3.	1	5	CW, QS	
9	**IWS 7** Further improving of nickel electroplating model. Modelling of electrolyte composition effect and/or electrode geometry.	LO 3	ID 3.3.		10	IT	
10	**L.10** Electrodeposition of metals at forced convection condition.	LO 4	ID 4.1.	1			Offline/traditional
10	**PT 10** Modelling of copper electrodeposition in rotating cylinder Hull cell type reactors	LO 4	ID 4.1.	2	15	TK and/or IT	
10	**MT (Midterm Exam)**	LO 3 - LO 4	ID 3.2. - ID 4.1.		100		
11	**L.11** Benefits of mass transport effect (hydrodynamic effect) on metal recovery by electrochemical methods	LO 4	ID 4.2.	1			Offline/traditional
11	**PT 11** Modelling of copper electrodeposition in rotating cylinder Hull cell (RCHC). Influence of diffusion layer thickness and/or electrode geometry.	LO 4	ID 4.2.	2	10	TK and/or IT	
11	IWSP 8 Consultation on the implementation of IWS8	LO 4	ID 4.2.	1	2	CW, QS	
11	**IWS 8** Advantages of RCHC type reactors on electrosynthesis application. Discussion of scientific article. Oral presentation.	LO 4	ID 4.2.		8	IT	
Module III							
12	**L.12** Introduction to modelling of chemical power sources.	LO 4	ID 4.3.	1			Offline/traditional
12	**PT 12** Modelling of discharge and self-discharge of lead-acid battery	LO 4	ID 4.3.	2	12	TK and/or IT	
12	**IWS 5** The processes occurring at charge/discharge of lead-acid battery discussion in detail. Oral presentation.	LO 4	ID 4.3.		5	IT	
13	**L.13** Influence of electrode material composition on self-discharge of lead-acid battery	LO 5	ID 5.1.	1			Offline/traditional
13	**PT 13** Modelling of discharge and self-discharge of lead-acid battery	LO 5	ID 5.1.	2	15	TK and/or IT	
13	IWSP 10 Consultation on the implementation of IWS10	LO 5	ID 5.1.	1		CW, QS	
13	**IWS 10** Rechargeable power sources. Oral presentation.	LO 5	ID 5.1.		5	IT	
14	**L.14** Electrochemistry of the lithium-ion battery	LO 5	ID 5.2.	1			Offline/traditional
14	**PT 14** Modelling of lithium-ion battery	LO 5	ID 5.2.	2	15	TK and/or IT	
14	**IWS 11** Lithium-ion batteries. Discussion of an article. Presentation.	LO 5	ID 5.2.		5	IT	
15	**L.15** Modelling of lithium-ion batteries in COMSOL Multiphysics using Lithium-ion battery Interface	LO 5	ID 5.3.	1			Offline/traditional
15	**PT 15** Modelling of lithium-ion battery	LO 5	ID 5.3.	2	15	TK and/or IT	

15	IWSP 12 Consultation on the implementation of IWS12	LO 5	ID 5.3.	1		CW, QS	
15	**IWS 12** Modelling of lithium-ion battery	LO 5	ID 5.3.		5	IT	
	MT 2	LO 4 - LO 5	ID 4.3. – ID 5.3.		100		

[Abbreviations: QS - questions for self-examination; TK - typical tasks; IT - individual tasks; CW - control work; MT - midterm.

Comments:

- Form of L and PT: webinar in MS Teams / Zoom (presentation of video materials for 10-15 minutes, then its discussion / consolidation in the form of a discussion / problem solving / ...)
- Form of carrying out the CW: webinar (at the end of the course, the students pass screenshots of the work to the monitor, he/she sends them to the teacher) / test in the Moodle DLS.
- All course materials (L, QS, TK, IT, etc.) see here (see Literature and Resources, p. 6).
- Tasks for the next week open after each deadline.
- CW assignments are given by the teacher at the beginning of the webinar.]

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