SYLLABUS
Fall semester 2024-2025 academic year Educational program
"6B07102 – Chemical Engineering"

ID and name of the course	Independent work of the student (IWS)	Number of credits			General number of credits	Independent work of the student under the guidance of a teacher (IWST)
		Lectures (L)	Seminars (S)	Lab. classes (LC)		
101773 Modeling of chemico-technological processes	2	1.5	4.5	-	6	7

ACADEMIC INFORMATION ABOUT THE COURSE

Learning Format	Cycle, component	Lecture types	Types of practical classes	Form and platform final control
Offline	CD, elective component	Analytical	Mixed	Written exam Offline System Univer
Lecturer	Khaisa Avchukir			
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ACADEMIC COURSE PRESENTATION

Purpose of the course	Expected Learning Outcomes (LO) *	Indicators of LO achievement (ID)
To learn the modelling of chemico-technological processes	1. Understand the importance of modeling in chemical engineering	1.1 Know the possible applications of the modeling in chemical engineering
		1.2 Understand the capabilities and limitations of modern modeling tools for chemical engineering
	2. Understand fundamental concepts of the modeling in chemical engineering	2.1 Know the theory of main physical and chemical processes
		2.2 To calculate mass and energy balances
	3. Build analytical and empirical models of chemico-technological processes	3.1 Know the principles of analytical and empirical modeling
		3.2 Obtain and use analytical equations
		3.3 Obtain and use empirical and semi-empirical equations
	4. Develop numerical models of chemico-technological processes	4.1 Know and understand principles of numerical modeling
		4.2 Use basic functions of COMSOL Multiphysics platform
		4.3 Model chemical reactions
		4.4 Model general electrochemical processes
		4.5 Model mass transport and partitioning of chemical species in homogeneous and heterogeneous media
		4.6 Model hydro-electrometallurgical processes
		4.7 Model chemical power sources
	5. Model complex processes	5.1 Model electrodeposition of metals onto massive surfaces
		5.2 Model real industrial processes
Prerequisites	General chemistry, Physical chemistry	
Postrequisites	No	

Learning Resources	**Literature:** 1. Finlayson B.A. Introduction to Chemical Engineering Computing. Second Edition. - John Wiley & Sons, 2012. ISBN 9781118309599, DOI: 10.1002/9781118309599 Pereira A.C., Inacio M., Pereira H., Paiva I. Modelling in Science and Engineering: A brief introduction to COMSOL Multiphysics 5. - Independently published, 2019. – 255 p. ISBN 1795702346 2. Pryor R.W. Multiphysics Modeling Using COMSOL5 and MATLAB. - Mercury Learning and Information, 2015. – 700 p. ISBN 1938549988 3. Ghasem N. Modeling and Simulation of Chemical Process Systems. - CRC Press, 2015. – 518 p. ISBN 1138568511 4. Gatzke E. Introduction to Modeling and Numerical Methods for Biomedical and Chemical Engineers. – Springer, 2021. – ISBN 3030764486 5. Chemical Reaction Engineering Module User's Guide. – COMSOL, 2020. 6. COMSOL Learning Center. – URL: https://www.comsol.com/learning-center/using-the-software-and-modeling-help-resources-from-comsol **Research infrastructure** 1. Computer and laboratory rooms at the Faculty of Chemistry and Chemical Technology 2. COMSOL Multiphysics 5.6 with Chemical Reaction Engineering Module **Professional scientific databases** 1. NIST Chemistry webbook, https://webbook.nist.gov/chemistry/ 2. SciFinder, https://scifinder.cas.org 3. UFZ-LSER database, https://www.ufz.de/index.php?de=31698&contentonly=1&m=0&lserd_data[mvc]=Public/start **Internet resources** 1. Web of Science, https://webofscience.com 2. Scopus, https://scopus.com 3. Google Scholar, https://scholar.google.com 4. Mendeley, https://www.mendeley.com 5. ResearchGate, https://www.researchgate.net **Software** 1. Microsoft Excel 2. COMSOL Multiphysics 5.6 with Chemical Reaction Engineering Module

Academic course policy	The academic policy of the course is determined by the Academic Policy and the Policy of Academic Integrity of Al-Farabi Kazakh National University . Documents are available on the main page of IS Univer. **Integration of science and education.** The research work of students, undergraduates and doctoral students is a deepening of the educational process. It is organized directly at the departments, laboratories, scientific and design departments of the university, in student scientific and technical associations. Independent work of students at all levels of education is aimed at developing research skills and competencies based on obtaining new knowledge using modern research and information technologies. A research university teacher integrates the results of scientific activities into the topics of lectures and seminars (practical) classes, laboratory classes and into the tasks of the IWST, IWS, which are reflected in the syllabus and are responsible for the relevance of the topics of training sessions and assignments. **Attendance.** The deadline for each task is indicated in the calendar (schedule) for the implementation of the content of the course. Failure to meet deadlines results in loss of points. **Academic honesty.** Practical/laboratory classes, IWS develop the student's independence, critical thinking, and creativity. Plagiarism, forgery, the use of cheat sheets, cheating at all stages of completing tasks are unacceptable. Compliance with academic honesty during the period of theoretical training and at exams, in addition to the main policies, is regulated by the "Rules for the final control" , "Instructions for the final control of the autumn / spring semester of the current academic year" , "Regulations on checking students' text documents for borrowings". Documents are available on the main page of IS Univer. **Basic principles of inclusive education.** The educational environment of the university is conceived as a safe place where there is always support and equal attitude from the teacher to all students and students to each other, regardless of gender, race / ethnicity, religious beliefs, socio-economic status, physical health of the student, etc. All people need the support and friendship of peers and fellow students. For all students, progress is more about what they can do than what they can't. Diversity enhances all aspects of life. All students, especially those with disabilities, can receive counseling assistance by phone / e- mail +77077090930/avchukir.khaisa@kaznu.edu.kz **Integration MOOC (massive open online course).** In the case of integrating MOOC into the course, all students need to register for MOOC. The deadlines for passing MOOC modules must be strictly observed in accordance with the course study schedule. **ATTENTION!** The deadline for each task is indicated in the calendar (schedule) for the implementation of the content of the course, as well as in the MOOC. Failure to meet deadlines results in loss of points.

INFORMATION ABOUT TEACHING, LEARNING AND ASSESSMENT

Score-rating letter system of assessment of accounting for educational achievements

Grade	Digital equivalent points	points, % content	Assessment according to the traditional system
A	4.0 _	95-100	Great
A-	3.67	90-94	
B+	3.33	85-89	Fine
B	3.0	80-84	
B-	2.67	75-79	
C+	2.33	70-74	
C	2.0	65-69	Satisfactorily
C-	1.67	60-64	
D+	1.33	55-59	
D	1.0	50-54	
FX	0,5	25-49	Unsatisfactory
F	0	0-24	

Assessment Methods

Criteria-based assessment is the process of correlating actual learning outcomes with expected learning outcomes based on clearly defined criteria. Based on formative and summative assessment.

Formative assessment is a type of assessment that is carried out in the course of daily learning activities. It is the current measure of progress. Provides an operational relationship between the student and the teacher. It allows you to determine the capabilities of the student, identify difficulties, help achieve the best results, timely correct the educational process for the teacher. The performance of tasks, the activity of work in the classroom during lectures, seminars, practical exercises (discussions, quizzes, debates, round tables, laboratory work, etc.) are evaluated. Acquired knowledge and competencies are assessed.

Summative assessment - type of assessment, which is carried out upon completion of the study of the section in accordance with the program of the course. Conducted 3-4 times per semester when performing IWS. This is the assessment of mastering the expected learning outcomes in relation to the descriptors. Allows you to determine and fix the level of mastering the course for a certain period. Learning outcomes are evaluated.

Formative and summative assessment	Points % content
Seminars	23.4
Independent work	18
Assessments	18.6
Final control (exam)	40
TOTAL	100

Calendar (schedule) for the implementation of the content of the course. Methods of teaching and learning.			
A week	**Topic name**	**Number of hours**	**Max. points**
MODULE 1 Fundamental concepts and basic modeling in chemical engineering.			
1	**L 1.** Introduction to the modeling in chemical engineering	1	-
	S 1. Discussion of possible applications of the modeling in chemical engineering	2	10
	IWS 1. Start of the work on preparing a basic computational model of a real process	4	-
2	**L 2.** Fundamental concepts of the modeling in chemical engineering	1	-
	S 2. Practice on calculating mass and energy balances	2	10
	IWST 1. Consultations on the implementation of **IWS 1**	1	-
	IWS 1. Further work on preparing a basic computational model of a real process	4	-
3	**L 3.** Analytical models of chemico-technological processes	1	-
	S 3. Practice on obtaining and using analytical equations	2	4
	IWST 2. Consultations on the implementation of **IWS 1**	1	-
	IWS 1. Further work on preparing a basic computational model of a real process	4	-
4	**L 4.** Empirical models of chemico-technological processes	1	-
	S 4. Practice on obtaining and using empirical equations	1	5
	A 1. Assessment 1	1	10
	IWS 1. Further work on preparing a basic computational model of a real process	4	-
MODULE 2 Basics of numerical modeling			
5	**L 5.** Introduction to numerical modeling	1	-
	S 5. Practice on obtaining and using simple numerical models	2	5
	IWS 1. Further work on preparing a basic computational model of a real process	4	-
6	**L 6.** Basic functions of COMSOL Multiphysics platform	1	-
	S 6. Practice on using basic functions of COMSOL Multiphysics platform	2	7
	IWST 3. Consultations on the implementation of **IWS 1**	1	-
	IWS 1. Finalizing and submission of a first draft of basic computational model of a real process	4	-
7	**L 7.** Modeling of chemical reactions	1	-
	S 7. Practice on obtaining and using models of chemical reactions	1	3
	A 2. Assessment 2	1	16
	IWS 1. Preparation and submission of a revised basic computational model of a real process	4	30
Midterm control 1			**100**
MODULE 3 Numerical modeling of physical and chemical processes			
8	**L 8.** Modeling of electrochemical processes	1	-
	S 8. Practice on obtaining and using models of electrochemical processes	2	5
	IWST 4. Consultations on the implementation of **IWS 2**	1	-
	IWS 2. Start of the work on preparing an advanced computational model of a real process	4	-
9	**L 9.** Modelling of a mass transport of chemical species in homogeneous media	1	-
	S 9. Practice on obtaining and using models for a mass transport of chemical species in homogeneous media	2	5
	IWS 2. Further work on preparing an advanced computational model of a real process	4	-
10	**L 10.** Modelling of general electrochemical processes and electrochemical methods of research	1	-
	S 10. Practice on obtaining and using models for a cyclic voltammetry and electrochemical impedance spectroscopy	2	8
	IWST 5. Consultation on the implementation **of IWS 2**	1	-
	IWS 2. Further work on preparing an advanced computational model of a real process	4	-
11	**L 11.** Modelling of a mass transport of chemical species in heterogeneous media	1	-
	S 11. Practice on obtaining and using models for a mass transport of chemical species in heterogeneous media	1	3
	A 3. Assessment 3	1	15
	IWS 2. Further work on preparing an advanced computational model of a real process	4	-
MODULE 4 Modeling of industrial processes			
12	**L 12.** Modeling of chemical power sources	1	-
	S 12. Practice on obtaining and using models for lead-acid batteries	2	7
	IWST 6. Consultation on the implementation **of IWS 2**	1	-
	IWS 2. Further work on preparing an advanced computational model of a real process	4	-
13	**L 13.** Modelling of hydro-electrometallurgical processes	1	-
	S 13. Practice on obtaining and using models for rotating cylinder Hull cell	2	7
	IWS 2. Further work on preparing an advanced computational model of a real process	4	-
14	**L 14.** Modelling of electrodeposition onto massive surfaces, types of the current distribution	1	-

	S 14. Practice on obtaining and using models for electrochemical coating of a car door	2	7
	IWS 2. Finalizing and submission of a first draft of an advanced computational model of a real process	4	-
15	**L 15.** Modelling of complex industrial processes	1	-
	S 15. Discussion on obtaining and using models for real industrial processes	1	3
	A 4. Assessment 4	1	10
	IWST 7. Consultation on the implementation **of IWS 2**	1	-
	IWS 2. Preparation and submission of a revised advanced computational model of a real process	4	30
Midterm control 2			**100**
Final control (exam)			**100**
TOTAL for course			**100**

Dean _____ **A.K. Galeyeva**

Chair of the Academic Committee
on the Quality of Teaching and Learning _____ **Bektemisova A.**

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Lecturer _____ **K. Avchukir**