

## COURSE OUTLINE

### (1) GENERAL

<b>SCHOOL</b>	School of Sciences		
<b>DEPARTMENT</b>	Department of Chemistry		
<b>LEVEL OF STUDIES</b>	ISCED level 6 – Bachelor's or equivalent level		
<b>COURSE CODE</b>	EN25	<b>SEMESTER</b>	7 or 8
<b>COURSE TITLE</b>	Chemical Process Modelling and Simulation		
<b>TEACHING ACTIVITIES</b> <i>If the ECTS Credits are distributed in distinct parts of the course e.g. lectures, labs etc. If the ECTS Credits are awarded to the whole course, then please indicate the teaching hours per week and the corresponding ECTS Credits.</i>		<b>TEACHING HOURS PER WEEK</b>	<b>ECTS CREDITS</b>
-		3	3
<i>Please, add lines if necessary. Teaching methods and organization of the course are described in section 4.</i>		-	-
<b>COURSE TYPE</b> <i>Background, General Knowledge, Scientific Area, Skill Development</i>	Specific Area		
<b>PREREQUISITES:</b>	No		
<b>TEACHING &amp; EXAMINATION LANGUAGE:</b>	Greek		
<b>COURSE OFFERED TO ERASMUS STUDENTS:</b>	Yes		
<b>COURSE URL:</b>	<a href="https://chem.duth.gr/en/courses/chemical-process-modelling-and-simulation">https://chem.duth.gr/en/courses/chemical-process-modelling-and-simulation</a>		

### (2) LEARNING OUTCOMES

<b>Learning Outcomes</b> <i>Please describe the learning outcomes of the course: Knowledge, skills and abilities acquired after the successful completion of the course.</i>
<p>After the successful completion of the course, participants will be able to:</p> <ul style="list-style-type: none"> <li>• Demonstrate advanced knowledge in the field of chemical process modeling and simulation.</li> <li>• Possess advanced cognitive and practical skills for solving complex and unpredictable problems encountered in the chemical industry.</li> <li>• Apply advanced techniques and methodologies for decision-making in highly demanding industrial environments.</li> </ul> <p><b>Knowledge</b></p> <ul style="list-style-type: none"> <li>• Understand the operation of major large-scale raw material processing units in the chemical industry.</li> <li>• Comprehend the principles of chemical engineering and industrial-scale process engineering.</li> <li>• Understand the fundamental principles and theories underlying process modeling methodologies.</li> </ul>

- Demonstrate knowledge of the reactions and reaction mechanisms involved in established chemical processes of the chemical industry.

### Skills

- Design and develop advanced process engineering algorithms.
- Design and analyze industrial process flow diagrams.
- Perform mass and energy balance calculations for chemical processes.
- Model and simulate real chemical processes for analysis, evaluation, and optimization purposes.
- Integrate and operate specialized laboratory equipment and advanced scientific simulators.
- Interpret production data and process information to effectively validate and improve process models.

### Abilities

- Supervise and manage the operation of industrial units in real time.
- Detect, diagnose, and efficiently resolve malfunctions, failures, and operational deficiencies in industrial facilities by selecting the most appropriate methodologies.
- Make informed decisions in complex industrial and engineering environments.
- Select appropriate instruments, analytical techniques, and combinations of methodologies for the monitoring and control of industrial chemical processes, taking into account both cost and effectiveness.
- Collaborate effectively with multidisciplinary teams of scientists and professionals in the international chemical industry to develop solutions to industrial process and engineering challenges.

### General Skills

*Name the desirable general skills upon successful completion of the module*

*Search, analysis and synthesis of data and information,*

*ICT Use*

*Adaptation to new situations*

*Decision making*

*Autonomous work*

*Teamwork*

*Working in an international environment*

*Working in an interdisciplinary environment*

*Production of new research ideas*

*Project design and management*

*Equity and Inclusion*

*Respect for the natural environment*

*Sustainability*

*Demonstration of social, professional and moral responsibility and sensitivity to gender issues*

*Critical thinking*

*Promoting free, creative and inductive reasoning*

The general skills that participants will have acquired upon successful completion of the module are:

- Search, analysis and synthesis of data and information, ICT use
- Adaptation to new situations
- Decision making
- Autonomous work
- Teamwork
- Working in an international environment
- Working in an interdisciplinary environment
- Production of new research ideas
- Project design and management
- Respect for the natural environment

- Sustainability
- Critical thinking
- Promoting free, creative and inductive reasoning

### (3) COURSE CONTENT

#### THEORY

- Fundamental Phase Equilibrium Calculations: Ideal and non-ideal mixtures.
- Equations of State (van der Waals, Peng–Robinson, Soave–Redlich–Kwong).
- Mass and Energy Balances.
- Degrees of Freedom Analysis: Simple and complex processes.
- Solution of Nonlinear Models (Newton, Lee, Christensen, and Rudd methods).
- Phase Diagrams and PVT Analysis.
- Process Modeling.
- Dynamic Process Simulation: Design and Development.
- Project Design and Development: Design of a pilot-scale chemical process unit and development of its simulation model.
- Mass and Energy Balance Studies: Development, analysis, and interpretation of multiple balances in a simulated chemical processing plant.
- Development of Process Logic and Advanced Algorithms for the Optimization of Chemical Industrial Units.
- Creation and Appropriate Use of Pseudocomponents (Hypotheticals/Pseudos): Understanding, development, and application of hypothetical components in complex process streams and mixtures.
- Use of Interactive Computational Tools: Understanding the contribution and effective utilization of the interactive calculation tools available within the simulation environment.
- Fault Detection Methodology: Development of troubleshooting methodologies, including the identification and resolution of process malfunctions, operational failures, omissions, and simulation over-parameterization issues.

### (4) LEARNING & TEACHING METHODS - EVALUATION

<b>TEACHING METHOD</b> <i>Face to face, Distance learning, etc.</i>	Face to face	
<b>USE OF INFORMATION &amp; COMMUNICATIONS TECHNOLOGY (ICT)</b> <i>Use of ICT in Teaching, in Laboratory Education, in Communication with students</i>	Use ICT in teaching and in communication with students: <ul style="list-style-type: none"> <li>• Digital slides</li> <li>• Scientific simulators</li> <li>• Videos</li> <li>• MS Teams / eclass, webmail</li> </ul>	
<b>TEACHING ORGANIZATION</b> <i>The ways and methods of teaching are described in detail. Lectures, Seminars, Laboratory Exercise, Field Exercise, Bibliographic research &amp; analysis, Tutoring, Internship (Placement), Clinical Exercise, Art Workshop, Interactive learning, Study visits, Study / creation, project, creation, project. Etc.</i>	<b>Activity</b>	<b>Workload/semester</b>
	Lectures	39
	Interactive learning	30
	Bibliographic research and analysis	21
	<b>Total</b>	<b>90</b>

<p><i>The supervised and unsupervised workload per activity is indicated here, so that total workload per semester complies to ECTS standards.</i></p>	
<p><b>STUDENT EVALUATION</b>  <i>Description of the evaluation process</i></p> <p><i>Assessment Language, Assessment Methods, Formative or Concluding, Multiple Choice Test, Short Answer Questions, Essay Development Questions, Problem Solving, Written Assignment, Essay / Report, Oral Exam, Presentation in audience, Laboratory Report, Clinical examination of a patient, Artistic interpretation, Other/Others</i></p> <p><i>Please indicate all relevant information about the course assessment and how students are informed</i></p>	<p>Student assessment is conducted through a written examination. The final written examination includes multiple-choice questions, short-answer questions, critical thinking questions, matching exercises, true/false questions, and problem-solving tasks carried out both in written form and in silico.</p> <p>The language of assessment is Greek.</p> <p>The evaluation criteria are communicated from the beginning of the course and are accessible to students via eclass.</p>

## (5) SUGGESTED BIBLIOGRAPHY

<p>- Recommended bibliography:</p> <ol style="list-style-type: none"> <li>1. Chemical Process Design and Simulation, J. Haydary, John Wiley &amp; Sons, 2019, ISBN: 9781119089117.</li> <li>2. Ανάλυση Χημικών Διεργασιών, Ι. Κούκος, 1η Έκδοση, 2010, ISBN: 978-960-418-267-1.</li> </ol> <p>- Relevant scientific journals:</p> <ol style="list-style-type: none"> <li>1. Chemical Engineering and Processing: Process Intensification, Elsevier.</li> <li>2. Industrial &amp; Engineering Chemistry Research, ACS Publication.</li> <li>3. Computers &amp; Chemical Engineering, Elsevier.</li> </ol>
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