UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: CHEMICAL THERMODYNAMICS
Type: CORE COURSE
Degree: 344 - CHEMICAL ENGINEERING
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Year: 2
Main language: Spanish
Use of additional languages: English
Web site:

Code: 57710
ECTS credits: 6
Academic year: 2022-23
Group(s): 21
Duration: First semester
Second language:
English Friendly: Y
Bilingual: N

Lecturer: **ALFONSO ARANDA RUBIO** - Group(s): **21**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie/2ª planta	QUÍMICA FÍSICA	926051915	alfonso.aranda@uclm.es	Tuesday, Wednesday and Thursday. 12-14h

Lecturer: **MARIA REYES LOPEZ ALAÑON** - Group(s): **21**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie (segunda planta))	QUÍMICA FÍSICA	926052779	reyes.lopez@uclm.es	Tuesday and Wednesday: 10-12h Thursday: 17-19 h

Lecturer: **ALBERTO NOTARIO MOLINA** - Group(s): **21**

Building/Office	Department	Phone number	Email	Office hours
Edificio Marie Curie, primera planta	QUÍMICA FÍSICA	6347	alberto.notario@uclm.es	Monday, 10-13h.Tuesday and Wednesday 10-11h

2. Pre-Requisites

Not established

3. Justification in the curriculum, relation to other subjects and to the profession

This course is part of the subject "Applied Chemical Kinetics and Thermodynamics"
The feasibility of a chemical process, from an energetic point of view, is given by Thermodynamics. For this reason, in all chemical-industrial processes, knowledge of thermodynamic aspects is required. In most cases, the rate of chemical processes has to be taken i
Thermodynamics also provides information about the properties of solid, liquid or gaseous systems depending on the conditions of pressure, volume and temperature. It is a basic subject. Knowledge of Chemical Thermodynamics is of special interest in Heat Engine

4. Degree competences achieved in this course

Course competences

Code	Description
CB02	Apply their knowledge to their job or vocation in a professional manner and show that they have the competences to construct and justify arguments and solve problems within their subject area.
E02	Understanding and mastery of basic concepts about the general laws of mechanics, thermodynamics, fields and waves and electromagnetism and its application for the resolution of engineering problems.
E07	Knowledge of applied thermodynamics and heat transmission. Basic principles and their application to solving engineering problems.
E24	Knowledge and / or ability to handle chemical analysis equipment and property characterization, and the basic instruments of a chemical laboratory.
E25	Knowledge about integration of processes and operations
E31	Ability to manage information sources in chemical engineering. Properly handle the terminology of the profession in Spanish and English in the oral and written records
G03	Ability to solve problems with initiative, decision making, creativity, critical reasoning and to communicate and transmit knowledge, skills and abilities in the field of Chemical Engineering.
G20	Ability to learn and work autonomously
G21	Ability to apply theoretical knowledge to practice
G22	Creativity and initiative

5. Objectives or Learning Outcomes

Course learning outcomes

Description
To know the methods based on generalized correlations.
To have the ability to autonomously work in a laboratory and skills in handling experimental techniques to obtain thermodynamic properties and the monitoring of kinetic processes.
To have knowledge and ability to manage bibliographic sources of thermodynamic and kinetic nature.
To have the skills to assess the viability of a chemical process from the thermodynamic point of view.
To have the skills to obtain the equilibrium constant for homogeneous and heterogeneous systems and to obtain the equilibrium concentrations under different pressure, temperature or reactive conditions.
To be able to calculate the (P,V,T) properties of real fluids.
To be able to calculate the activity coefficients of the chemical species involved in non ideal systems
To have the skills to understand and build phase equilibrium diagrams for non ideal systems
To be able to understand and build tables and grafics of thermodynamic properties of real fluids.

6. Units / Contents

Unit 1: Introduction to Thermodynamics

Unit 2: First Law of Thermodynamics. Internal energy and enthalpy. Cp and Cv. Calculations of heat, work, increases in U and H for ideal gases in different reversible and irreversible processes. Joule-Thompson experiment. Joule-Thompson coefficient. Applications.

Unit 3: Entropy. Second principle of Thermodynamics. Carnot cycle. Thermal machines and their performance. Third law of Thermodynamics. Calculation of entropy in different processes.

Unit 4: Free energy functions and material equilibrium criteria. spontaneity criteria. Relations between thermodynamic functions. Gibbs equations and Maxwell relations. Calculations of increases of G, A, H, S, U in different thermodynamic processes. How to influence a non-spontaneous process to make it viable.

Unit 5: Thermochemistry. Definition of standard states. Formation enthalpies. Calculations of enthalpies, entropies and free energies of reaction. Table management. Effect of temperature. Adiabatic flame temperature.

Unit 6: Phase Equilibrium in Monocomponent Systems. Phase rule. Phase equilibrium diagrams. Critical point. Equilibrium between phases, Clapeyron equation. Clausius-Clapeyron equation.

Unit 7: Behavior of pure real gases and liquids. Real gases, behavior. Equations of state, virial, cubic and more complex. Principle of corresponding states, equations and generalized diagrams. Real gas mixtures. Liquid state, equations and methods. Applications to storage and transport of fluids.

Unit 8: Thermodynamic properties of real fluids. Residual magnitudes. Methods for calculating increases in thermodynamic magnitudes in real monocomponent systems and in mixtures. Fugacity.

Unit 9: Thermodynamics of Variable Composition Systems. Partial molar properties. Gibbs-Duhem equation. Mixing processes. ideal solutions. Equilibrium L-F. Construction of equilibrium diagrams L-V. Bubble point, dew point and fractionation calculations. Ideally diluted solutions. Colligative properties.

Unit 10: Phase equilibrium in real multicomponent systems. Definition of reference states. Activity coefficients and calculation of chemical potential. Mix and excess functions. Methods for calculating activity coefficients. Real L-V diagrams. Azeotropes. Bubble and dew points. Distillation. L-L-F equilibria. Distillation of partially miscible liquids. Ternary diagrams.

Unit 11: Chemical equilibrium in ideal and real systems. Reacting systems, reaction coordinate. Equilibrium constant in homogeneous systems. Equilibrium thermodynamics in heterogeneous systems. Variation of the equilibrium constant with P and T. Van't Hoff equation. Le Chatelier's principle. coupled reactions. Equilibriums with ions in solution.

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Class Attendance (practical) [ON-SITE]	Practical or hands-on activities	CB02 E07 E24 E25 G20 G22	0.65	16.25	Y	Y	
Class Attendance (theory) [ON-SITE]	Lectures	E02 E07 E25 E31 G03 G20 G21 G22	1.3	32.5	Y	N	
Workshops or seminars [ON-SITE]	Workshops and Seminars	CB02 E07 E25 E31 G20 G21 G22	0.35	8.75	Y	Y	
Practicum and practical activities report writing or preparation [OFF-SITE]	Group Work	E07 E25 G21 G22	0.32	8	Y	Y	
Writing of reports or projects [OFF-SITE]	Group Work	E07 G03 G20 G22	0.16	4	Y	N	
Final test [ON-SITE]	Assessment tests	E07 E24 E25 G20 G22	0.1	2.5	Y	Y	
Study and Exam Preparation [OFF-SITE]	Combination of methods	E07 G03 G20 G21 G22	3.12	78	N	-	
		Total:	**6**	**150**			
		Total credits of in-class work: 2.4					**Total class time hours: 60**
		Total credits of out of class work: 3.6					**Total hours of out of class work: 90**

As: Assessable training activity
Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Final test	60.00%	60.00%	
Laboratory sessions	10.00%	10.00%	
Practicum and practical activities reports assessment	5.00%	5.00%	
Assessment of problem solving and/or case studies	25.00%	25.00%	
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

1. exam with questions and problems about the contents studied in the subject (60% of the grade)
2. Continuous evaluation of laboratory work (15%) including the writing of a report with the results sheets.
3. Continuous evaluation on problem-based learning, especially during seminar hours (25%). The student will be asked to deliver solved exercises, solve different questions related to the subject, resolution of practical cases, group work, etc.
To pass the subject, in both the exam and in the practices, a minimum of 4.0/10 will be required and the average must be equal to or greater than 5.0/10.

Non-continuous evaluation:

1. Exam with questions and problems about the contents studied in the subject (85%)
2. Laboratory exam (15%). Performance of experimental work, questionnaire and report of results.

Specifications for the resit/retake exam:

1. Evaluation of the work in the laboratory (15%) including the preparation of the results sheets. The laboratory score (from te continuous evaluation)is kept for all students. For those who have not passed the threshold of 4.0 in the ordinary call or wish to be evaluated again, this call will have a section for the evaluation of the corresponding skills that could be carried out in the laboratory.
2. exam with questions and problems similar to those found in the seminar classes on the contents studied in the subject, 85%. To pass the subject it is required to obtain a minimum of 4 in this test and an average equal to or greater than 5.

Specifications for the second resit / retake exam:

1. Evaluation of the work in the laboratory (15%) including the preparation of the results sheets. The laboratory score (from te continuous evaluation)is kept for all students. For those who have not passed the threshold of 4.0 in the ordinary call or wish to be evaluated again, this call will have a section for the evaluation of the corresponding skills that could be carried out in the laboratory.
2. exam with questions and problems similar to those found in the seminar classes on the contents studied in the subject, 85%. To pass the subject it is required to obtain a minimum of 4 in this test and an average equal to or greater than 5.

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	hours

Unit 1 (de 11): Introduction to Thermodynamics

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	.5
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	2

Unit 2 (de 11): First Law of Thermodynamics. Internal energy and enthalpy. Cp and Cv. Calculations of heat, work, increases in U and H for ideal gases in different reversible and irreversible processes. Joule-Thompson experiment. Joule-Thompson coefficient. Applications.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	5

Unit 3 (de 11): Entropy. Second principle of Thermodynamics. Carnot cycle. Thermal machines and their performance. Third law of Thermodynamics. Calculation of entropy in different processes.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	5

Unit 4 (de 11): Free energy functions and material equilibrium criteria. spontaneity criteria. Relations between thermodynamic functions. Gibbs equations and Maxwell relations. Calculations of increases of G, A, H, S, U in different thermodynamic processes. How to influence a non-spontaneous process to make it viable.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	2.5
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	6

Unit 5 (de 11): Thermochemistry. Definition of standard states. Formation enthalpies. Calculations of enthalpies, entropies and free energies of reaction. Table management. Effect of temperature. Adiabatic flame temperature.

Activities	Hours
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	3.5
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Practicum and practical activities report writing or preparation [AUTÓNOMA][Group Work]	1
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	8

Unit 6 (de 11): Phase Equilibrium in Monocomponent Systems. Phase rule. Phase equilibrium diagrams. Critical point. Equilibrium between phases, Clapeyron equation. Clausius-Clapeyron equation.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	7

Unit 7 (de 11): Behavior of pure real gases and liquids. Real gases, behavior. Equations of state, virial, cubic and more complex. Principle of corresponding states, equations and generalized diagrams. Real gas mixtures. Liquid state, equations and methods. Applications to storage and transport of fluids.

Activities	Hours
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	3.5
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Practicum and practical activities report writing or preparation [AUTÓNOMA][Group Work]	1
Writing of reports or projects [AUTÓNOMA][Group Work]	4
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9

Unit 8 (de 11): Thermodynamic properties of real fluids. Residual magnitudes. Methods for calculating increases in thermodynamic magnitudes in real monocomponent systems and in mixtures. Fugacity.

Activities	Hours
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	3
Class Attendance (theory) [PRESENCIAL][Lectures]	3
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Practicum and practical activities report writing or preparation [AUTÓNOMA][Group Work]	2
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9

Unit 9 (de 11): Thermodynamics of Variable Composition Systems. Partial molar properties. Gibbs-Duhem equation. Mixing processes. ideal solutions. Equilibrium L-F. Construction of equilibrium diagrams L-V. Bubble point, dew point and fractionation calculations. Ideally diluted solutions. Colligative properties.

Activities	Hours
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	3
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Practicum and practical activities report writing or preparation [AUTÓNOMA][Group Work]	2
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9

Unit 10 (de 11): Phase equilibrium in real multicomponent systems. Definition of reference states. Activity coefficients and calculation of chemical potential. Mix and excess functions. Methods for calculating activity coefficients. Real L-V diagrams. Azeotropes. Bubble and dew points. Distillation. L-L-F equilibria. Distillation of partially miscible liquids. Ternary diagrams.

Activities	Hours
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9

Unit 11 (de 11): Chemical equilibrium in ideal and real systems. Reacting systems, reaction coordinate. Equilibrium constant in homogeneous systems. Equilibrium thermodynamics in heterogeneous systems. Variation of the equilibrium constant with P and T. Van't Hoff equation. Le Chatelier's principle. coupled reactions. Equilibriums with ions in solution.

Activities	Hours
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	3.25
Class Attendance (theory) [PRESENCIAL][Lectures]	5.5
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	1.75
Practicum and practical activities report writing or preparation [AUTÓNOMA][Group Work]	2
Final test [PRESENCIAL][Assessment tests]	2.5
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	9

Global activity

Activities	hours
Class Attendance (practical) [PRESENCIAL][Practical or hands-on activities]	16.25
Class Attendance (theory) [PRESENCIAL][Lectures]	32.5
Workshops or seminars [PRESENCIAL][Workshops and Seminars]	8.75
Practicum and practical activities report writing or preparation [AUTÓNOMA][Group Work]	8
Writing of reports or projects [AUTÓNOMA][Group Work]	4
Final test [PRESENCIAL][Assessment tests]	2.5
Study and Exam Preparation [AUTÓNOMA][Combination of methods]	78
Total horas:	150

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Yunus A. Cengel, Michael A. Boles y Mehmet Kanoglu	Termodinámica	Mc. Graw Hill		9 781456 27208	2019	
Felder, Richard M.	Elementary principles of chemical processes	Wiley		978-0-471-37587-6	2005	
Levine, Ira N.	Fisicoquímica (principios de)	McGraw-Hill		978-607-15-0988-8	2014	
Moran, Michael J.	Fundamentos de termodinámica técnica	Reverté		84-291-4313-0	2004	
Poling, Bruce E.	The properties of gases and liquids	McGraw-Hill		0-07-011682-2	2001	
Sandler, Stanley I.	Chemical, Biochemical, and Engineering Thermodynamics, 5th Edition	John Wiley & Sons		978-0-470-50479-6	2017	
Smith, Joe M.	Introducción a la termodinámica en ingeniería química	McGraw-Hill		978-1-47722-2	2020	
Wark, Kenneth	Termodinamica	McGraw-Hill		84-481-2829-X	2001	