# SUBJECT TEACHING GUIDE

## G792 - Further Thermodynamics

## Degree in Chemical Engineering
## First Degree in Chemical Engineering

Academic year 2024-2025

| 1. IDENTIFYING DATA | | | | | |
|---|---|---|---|---|---|
| Degree | Degree in Chemical Engineering<br>First Degree in Chemical Engineering | | Type and Year | Optional. Year 4<br>Optional. Year 4 | |
| Faculty | School of Industrial Engineering and Telecommunications | | | | |
| Discipline | Subject Area: Option A: Fundamental Chemical Engineering<br>Optional Module | | | | |
| Course unit title and code | G792 - Further Thermodynamics | | | | |
| Number of ECTS credits allocated | 6 | Term | Semester based (2) | | |
| Web | | | | | |
| Language of instruction | Spanish | English Friendly | Yes | Mode of delivery | Face-to-face |

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|---|---|
| Department | DPTO. INGENIERIAS QUIMICA Y BIOMOLECULAR |
| Name of lecturer | MANUEL ALVAREZ GUERRA |
| E-mail | manuel.alvarezg@unican.es |
| Office | E.T.S. de Ingenieros Industriales y de Telecomunicación. Planta: - 2. DESPACHO PROFESORADO (S2011) |
| Other lecturers | EUGENIO DANIEL GORRI CIRELLA |

| 3.1 LEARNING OUTCOMES |
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| - To be able to use the thermodynamic principles of interest in the field of Chemical Engineering. |
| - To be able to apply classical thermodynamic models to describe the behaviour of pure fluids and simple mixtures. |
| - To be able to identify advanced thermodynamic models that are currently used to model complex systems. |
| - To be able to know different mathematical tools that are currently available to solve thermodynamic problems and to be able to apply them to answer to the usual needs that appear in the professional field of the chemical engineer. |

## 4. OBJECTIVES

To understand concepts, principles, relations and experimental basis of the thermodynamic theory that broaden those studied in previous subjects of the degree, from an essentially practical and applied point of view.
To go deeply into the practical application of classical thermodynamic models such as the cubic equations of state or activity coefficient models. To introduce the student to current and more advanced models based on statistical mechanics and molecular thermodynamics, which are of interest to describe the behaviour of complex fluids.
To solve practical cases that allow the students to know the possibilities that different computer tools could offer to tackle thermodynamic problems that they could need to use in their professional future: general software widely available (e.g. Excel), chemical processes simulators (e.g. Aspen Plus), specific software (e.g. COSMOtherm).

## 6. SUBJECT PROGRAM

| | CONTENTS |
|---|---|
| 1 | Review of basic thermodynamic aspects. Principles of phase equilibria. Chemical potential, fugacity. |
| 2 | Classical thermodynamic models: Fundamentals and practical applications using general software (Excel, MATLAB), chemical processes simulators (Aspen Plus) and specific software (Thermosolver, UNIFAC).<br>2.1. Cubic equations of state. Calculation of density of fluids and of fugacities. Extension to multicomponent mixtures.<br>2.2. Group contribution methods to estimate properties. Applications to the estimation of critical constants, densities, heat capacities, enthalpies of formation. Estimation of parameters of environmental interest with EPI Suite.<br>2.3. Activity coefficient models. Group contribution methods (UNIQUAC, UNIFAC).<br>2.4. Applications to phase equilibria calculations: (a) VLE: Fitting of experimental data to obtain activity coefficients; (b) LLE: Prediction of separation of phases and compositions at equilibrium; (c) Equilibrium in electrolyte solutions; (d) VLE at high pressures: bubble point, dew point, flash evaporation.<br>2.5. Chemical equilibrium: systems with multiple reactions. Equilibrium in heterogeneous systems.<br>2.6. Thermal and refrigeration cycles |
| 3 | Advanced thermodynamic models: introduction to the fundamentals and examples of practical applications<br>3.1. Basic concepts of statistical mechanics and molecular thermodynamics.<br>3.2. SAFT (Statistical Associating Fluid Theory) and CPA EoS (Cubic-Plus-Association Equation of State) models<br>3.3. Introduction to computer simulation methods: Molecular Dynamics and Monte Carlo Method.<br>3.4. Methods based on quantum mechanics calculations: COSMO-RS method. Practical applications using advanced software (COSMOtherm). |

| 7. ASSESSMENT METHODS AND CRITERIA | | | | |
|---|---|---|---|---|
| Description | Type | Final Eval. | Reassessn | % |
| Objective Test 1 | Written exam | No | Yes | 10,00 |
| Portfolio 1 | Work | No | Yes | 40,00 |
| Objective Test 2 | Written exam | No | Yes | 10,00 |
| Portfolio 2 | Work | No | Yes | 40,00 |
| TOTAL | | | | 100,00 |

Observations

The continuous assessment is based on carrying out two objective tests (weeks 8 and 15 of the four-month period) and carrying out and submitting two portfolios about the different activities and practical applications proposed . In order to be eligible for continuous assessment in the course, students must have attended 80% of the in-person classes.
Students who do not pass the course through continuous assessment will have the option to take the final exam on the dates established by the School.

Observations for part-time students

In the event that the part-time students cannot regularly participate in the teaching activities, they could undergo a single evaluation process consisting of the delivery of the portfolios in the ordinary examination period (80% of the final grade) and doing the final test on the date established by the Center (remaining 20%).

## 8. BIBLIOGRAPHY AND TEACHING MATERIALS

BASIC

J.R. Elliott, C.T. Lira. “Introductory Chemical Engineering Thermodynamics, 2nd ed.” Prentice Hall Pearson Education, New Jersey, 2012.

M. Koretsky, "Engineering and chemical thermodynamics", 2nd edition, Wiley, Hoboken, New Jersey, 2013.

J.R. Elliott, V.Diky, T.A. Knotts, W.V. Wilding. “The Properties of Gases and Liquids”, 6th ed., McGraw-Hill, New York, 2023.