

## SUBJECT TEACHING GUIDE

G792 - Further Thermodynamics

Degree in Chemical Engineering

Academic year 2017-2018

1. IDENTIFYING DATA					
Degree	Degree in Chemical Engineering			Type and Year	Optional. Year 4
Faculty	School of Industrial Engineering and Telecommunications				
Discipline	Subject Area: Option A: Fundamental Chemical Engineering 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	No	Mode of delivery	Face-to-face

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: - 5. DESPACHO (S5005)				
Other lecturers	EUGENIO DANIEL GORRI CIRELLA				

### 3.1 LEARNING OUTCOMES

- 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. COURSE ORGANIZATION

##### CONTENTS

1	Review of basic thermodynamic aspects. Principles of phase equilibria. Chemical potential, fugacity.
2	<p>Classical thermodynamic models: Fundamentals and practical applications using general software (Excel, MATLAB), chemical processes simulators (Aspen Plus) and specific software (Thermosolver, UNIFAC).</p> <p>2.1. Cubic equations of state. Calculation of density of fluids and of fugacities. Extension to multicomponent mixtures.</p> <p>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.</p> <p>2.3. Activity coefficient models. Group contribution methods (UNIQUAC, UNIFAC).</p> <p>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.</p> <p>2.5. Chemical equilibrium: systems with multiple reactions. Equilibrium in heterogeneous systems.</p>
3	<p>Advanced thermodynamic models: introduction to the fundamentals and examples of practical applications</p> <p>3.1. Basic concepts of statistical mechanics and molecular thermodynamics.</p> <p>3.2. SAFT (Statistical Associating Fluid Theory) and CPA EoS (Cubic-Plus-Association Equation of State) models</p> <p>3.3. Introduction to computer simulation methods: Molecular Dynamics and Monte Carlo Method.</p> <p>3.4. Methods based on quantum mechanics calculations: COSMO-RS method. Practical applications using advanced software (COSMOtherm).</p>

#### 7. ASSESSMENT METHODS AND CRITERIA

Description	Type	Final Eval.	Reassessn	%
Objective Test 1	Written exam	No	Yes	10,00
Portfolio 1	Work	No	Yes	30,00
Presentation Portfolio 1	Others	No	Yes	10,00
Objective Test 2	Written exam	No	Yes	10,00
Portfolio 2	Work	No	Yes	30,00
Presentation Portfolio 2	Others	No	Yes	10,00
<b>TOTAL</b>				<b>100,00</b>
<b>Observations</b>				
The continuous evaluation is based on carrying out two objective tests (weeks 8 and 15 of the four-month period) and the submission and oral presentation of two portfolios about the activities and practical applications proposed.				
<b>Observations for part-time students</b>				
The results obtained by part-time students will be maintained during one academic year.				

## 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.

B. Poling, J. M. Prausnitz, J. O'Connell. "The Properties of Gases and Liquids", 5th ed., McGraw-Hill, New York, 2001.