Course Unit	Chemical Thermodynamics I			Field of study	Thermodynamics and Transport Phenomena
Bachelor in	Chemical Engineering			School	School of Technology and Management
Academic Year	2022/2023	Year of study	2	Level	1-2	ECTS credits	6.0
Type	Semestral	Semester	1	Code	9125-755-2105-00-22		

Workload (hours)	162	Contact hours	T	TP	PL	TC	S	E	OT	O
			30	-	30	-	-	-	-	-

T - Lectures; TP - Lectures and problem-solving; PL - Problem-solving, project or laboratory; TC - Fieldwork; S - Seminar; E - Placement; OT - Tutorial; O - Other

Name(s) of lecturer(s): Simão Pedro de Almeida Pinho

Learning outcomes and competences

At the end of the course unit the learner is expected to be able to:
1. Recognize the importance of thermodynamics in the design, development and operation of processes, pursuing an efficient use of energy.
2. Explain and apply the laws of thermodynamics in several types of systems and processes, and evaluate the energetic needs in chemical processes.
3. Define and explain the ideality concept, and identify its relation with real systems and processes. Apply the laws of thermodynamics to define efficiency in processes.
4. Use and know experimental methods in the determination of thermodynamic properties of pure substances.
5. Analyse, interpret and apply experimental information in problems involving mass and energy balances.
6. Use experimental data for the thermodynamic description of a pure substance in conditions not available experimentally.
7. Explain the meaning of an equation of state and recognize their different forms, characteristics and potentialities.

Prerequisites

Before the course unit the learner is expected to be able to:
1. Apply general mathematics concepts, particularly differential and integral calculus.
2. Use informatic tools such as MATLAB or MS Excel.

Course contents

The first law of thermodynamics and other fundamental concepts. Volumetric properties of pure fluids. Thermal effects in chemical processes. Second law of thermodynamics. Thermodynamic properties of pure fluids. Thermodynamics of flow processes.

Course contents (extended version)

1. Introduction
   - Importance of thermodynamics. Dimensions and units. Fundamental concepts: system and surroundings.
   - Temperature scale, force, pressure and volume. Different forms of energy: heat and work.
2. First law of Thermodynamics and other Fundamental Concepts
   - Joule experiments. Definition of internal energy.
   - Mathematical expression for the first law.
   - State functions and enthalpy. First law applied to steady state flow processes.
   - Equilibrium state of a system and Gibbs phase rule.
   - Reversible processes. Constant volume or constant pressure processes. Heat capacities.
3. Volumetric Properties of Pure Fluids
   - PVT diagrams. Ideal gas concept. Virial equation and its applications.
   - Cubic equations of state: van der Waals, Redlich-Kwong and Peng-Robinson.
   - Physical meaning for the liquid and molar molar volumes using cubic EoS.
   - Correspondent states theorem. Generalized correlations for gases: Lee-Kesler and Pitzer.
   - Correlations for liquids: Lee-Kesler, method of Lydersen, Greenkorn e Hougen, and Rackett equation.
4. Thermal Effects in Chemical Processes
   - Heat capacities and its change with temperature. Phase change enthalpies: Clapeyron equation.
   - Riedel and Watson equations for heat of vaporization.
   - Standard enthalpies of formation, reaction and combustion. Temperature effect.
5. Second Law of Thermodynamics
   - Second law of thermodynamics. Heat machines. Carnot Cycle.
   - Thermodynamic and ideal gas temperature scales.
   - Entropy concept. Entropy changes in processes with ideal gases.
   - Mathematical expression for 2nd law. Entropy as equilibrium criterium. 3rd law of thermodynamics.
   - Thermodynamic analysis of processes: ideal and lost work, and efficiency.
   - Cycles for heat conversion into work.
6. Thermodynamic Properties of Pure Fluids
   - Two new thermodynamic properties: Gibbs and Helmholtz energies.
   - Relation between properties of homogeneous phases. Maxwell relations.
   - Expressions for the calculation of enthalpy and entropy as a function of temperature and pressure.
   - Expressions for the calculation of Gibbs and Helmholtz energies.
   - Residual properties. Two-phase systems.
   - Tables and diagrams for thermodynamic properties of gases and liquids.
   - Generalized correlations for the calculation of residual properties.
7. Flow processes thermodynamics
   - Control volume and surface. Balance equations: mass, energy, and entropy.
   - Thermodynamic analysis of processes. Calculation of ideal work and thermodynamic efficiency.
   - Relation between lost work and entropy generation. Internal and external irreversibility.
   - Flow of compressible fluids. Expansion and compression processes.

Recommended reading

1. J. M. Smith; H. C. Van Ness e M. M. Abbott, Introduction to Chemical Engineering Thermodynamics, 7th Edition, McGraw-Hill, 2005.
2. S. P. Pinho, Manual da Disciplina de Termodinâmica Química I, Escola Superior de Tecnologia e de Gestão, Bragança, 2006.
3. E. G. Azevedo, Termodinâmica Aplicada, 2ª Edição, Escolar Editora, 2000.
4. S. I. Sandler, Chemical and Engineering Thermodynamics, 3rd edition, John Wiley & Sons, 1999.
5. J. R. Elliot e C. T. Lira, Introductory Chemical Engineering Thermodynamics, Prentice-Hall, 1999.

Teaching and learning methods

Theoretical analysis of fundamental tools and concepts for the comprehension, application and calculations in the thermodynamics area. Presentation of practical

Teaching and learning methods

examples and exercises. Problem solving and critical analysis of the results. Evaluation of homework. Development of application projects.

Assessment methods

1. Alternative 1 - (Regular, Student Worker) (Final)
   - Projects - 10% (Development and critical analysis of selected problems.)
   - Intermediate Written Test - 45% (Partial written exam. Minimum grade: 6.)
   - Intermediate Written Test - 45% (Partial written exam.)
2. Alternative 2 - (Regular, Student Worker) (Final, Supplementary, Special)
   - Final Written Exam - 100% (Global written exam.)

Language of instruction

English

Electronic validation

Simão Pedro de Almeida Pinho	Hélder Teixeira Gomes	Ramiro José Espinheira Martins	Paulo Alexandre Vara Alves
13-10-2022	22-10-2022	22-10-2022	24-10-2022