UAB
Universitat Autònoma de Barcelona

Applied Thermodynamics

Code: 102442
ECTS Credits: 6

2024/2025

Degree	Type	Year
2500897 Chemical Engineering	OB	2

Contact

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

No official requirements are defined for this course. However, we strongly recommend that the student has passed the first year courses of Physics, Chemistry, Computer Applications and Balance in Chemical Engineering.

Objectives and Contextualisation

The principles of Thermodynamics and their application in Chemical Engineering are presented. From the formulation and discussion of thermodynamic principles, these are used to determine the properties of pure fluids and mixtures. A fundamental objective is the thermodynamic analysis of systems in equilibrium, both physical balance between phases, and the balance in systems with chemical reaction. In both cases, it is about the quantification and analysis of the balance for its future application in the design of reactors and unit operations.

Competences

Chemical Engineering
- Communication
- Develop personal work habits.
- Develop thinking habits.
- Understand and apply the basic principles on which chemical engineering is founded, and more precisely: balances of matter, energy and thermodynamic momentum, phase equilibrium and kinetic chemical equilibrium of the physical processes of matter, energy and momentum transfer, and kinetics of chemical reactions

Learning Outcomes

1. Apply the scientific and technological basics of thermodynamics, phase equilibrium and chemical equilibrium and the kinetics of physical energy transfer processes.

2. Communicate efficiently, orally and in writing, knowledge, results and skills, both professionally and to non-expert audiences.
3. Develop critical thinking and reasoning
4. Work autonomously.

Content

0.- Introduction

Thermodynamics. Thermodynamics and Chemical Engineering. Definitions and nomenclature. Thermodynamic properties. Equilibrium. Thermodynamic variables. Gibbs phase rule. PVT behavior.

1.- First principle of Thermodynamics and basic concepts

First principle. Internal energy. State functions. Enthalpy. Equilibrium. Gibbs Rule of phases. Reversible processes. Processes at constant volume and pressure. Specific heat. Isotherm, Adiabatic and Polytropic processes.

2.- Second principle of Thermodynamics. Entropy

Second principle. The thermal machine. Carnot cycle for an ideal gas. Entropy

3.- Volumetric and thermodynamic properties of fluids

Estimation of volumetric properties of pure fluids. P-V-T behavior of pure substances. Corresponding states theory. Critical properties. Compressibility factor. State equations. Generalized correlations for liquids. Relationships between thermodynamic properties. Gibbs energy. Residual properties.

4.- Thermochemistry

Heat determination . Methods of calculation of heat in phase changing. Entalpies of formation. Reaction Enthalpy.

5.- Evaluation of properties in multicomponent systems

Estimation of volumetric properties of mixtures. Mixing rules. Adaptation of the equations of state. Gibbs-Duhem equation. Partial molar properties. Chemical potential.

6.- Phase Equilibrium

Fugacity and fugacity coefficient. Activity and activity coefficient. Equilibrium criteria. Vapor Liquid equilibrium: ideal case. Behavior not ideal. Bubble point and dew point. Calculation of coefficients of fugacity or activity. Models for its calculation.

7.- Chemical Equilibrium

Equilibrium constant. Methods of calculating the equilibrium constant. Determination of the compositions in the equilibrium state.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			

Lectures	30	1.2	1
Problems	15	0.6	1, 3, 4
simulator	5	0.2	1, 2, 3, 4
Type: Autonomous			
Problems solving	47	1.88	1, 2, 3, 4
documentación y bibliografía	5	0.2	3, 4
study	35	1.4	1, 2, 3, 4

Guided activities:

Theoretical classes: Master classes on the topics of the syllabus.

Problem classes: solving problems related to the subject. Discuss with the students about the solution strategies and their execution.

Simulator use seminars: Presentation seminars for the use of process simulators in the estimation of thermodynamic properties and equilibrium compositions.

Autonomous activities:

Study: Individual study. Schemes and summaries preparation.

Problem solving: Self-solving problem solving. On the one hand, as a complement to the own study of the subject and, on the other, as a preliminary work to the classes of problems.

Use of process simulator to estimate properties and solve equilibrium problems between phases of multi-component systems.

Search for documentation and bibliography: Check the essential documentary resources for the course.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
First Test	40 %	3.5	0.14	1, 2, 3
Retaking exam	85%	5	0.2	1, 2, 3
Second test	45%	3.5	0.14	1, 2, 3
Simulation work	15%	1	0.04	1, 2, 3, 4

Evaluation by course:
1st partial test (PP1) (topics 1 to 5): 40% grade.
2nd partial test (PP2) (topics 6 and 7): 45% grade.
Work with process simulator: 15% note.
You have to obtain a 3/10 in the theoretical part of each partial test to get d'exam pass and 3/10 in each partial test to pass the subject per course.

Single assessment: those who accept the single assessment process by declaring it at the beginning of the course, will take the day of the second partial test, an additional part corresponding to the first part of the course.

Retaking exam:
There will be a final global test for those students who have not passed the continuous assessment (note <5).

See more details in Catalan guide

Bibliography

Koretsky, M.D. Engineering and Chemical Thermodynamics. John Wiley and Sons Ltd. USA. (2012)

Smith, J.M.; Van Ness, H.C. Introduction to Chemical Engineering Thermodynamics. 8th ed. McGraw-Hill Education. (2018).

Sandler, S.I. Chemical and Engineering Thermodynamics. 4th ed. Wiley, John Wiley and Sons Ltd. USA. (2007).

Moran, M.J.; Shapiro, H.N. Fundamentals of Engineering Thermodynamics. 6th ed. John Wiley and Sons Ltd. USA. (2007).

Software

Access to a chemical process simulator (HYSYS) will be given

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	211	Catalan	first semester	morning-mixed
(PAUL) Classroom practices	212	Catalan	first semester	morning-mixed
(SEM) Seminars	211	Catalan	first semester	morning-mixed
(SEM) Seminars	212	Catalan	first semester	morning-mixed
(TE) Theory	22	Catalan	first semester	morning-mixed