Universitat Autònoma de Barcelona

2019/2020

Applied Thermodynamics

Code: 102442
ECTS Credits: 6

Degree	Type	Year	Semester
2500897 Chemical Engineering	OB	2	2

Contact

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Use of Languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

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 and Balance in Chemical Engineering. Have studied or are studying Computer Applications is also recommended.

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

- Apply relevant knowledge of the basic sciences, such as mathematics, chemistry, physics and biology, and the principles of economics, biochemistry, statistics and material science, to comprehend, describe and resolve typical chemical engineering problems.
- Develop personal attitude.
- Develop personal work habits.
- Develop thinking habits.

Learning Outcomes

1. Apply relevant knowledge from the basic sciences, such as mathematics, physics and especially chemistry to understand, describe and resolve typical chemical engineering problems.
2. Develop a capacity for analysis, synthesis and prospection.
3. Develop curiosity and creativity.
4. Manage available time and resources. Work in an organised manner.

Content

0.- Introduction

Thermodynamics. Thermodynamics and Chemical Engineering. Definitions and nomenclature.

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. 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

P-V-T behavior of pure substances. Theory of the corresponding states. Critical properties. Acentric factor. Estimation of volumetric properties of pure fluids. Equations of state. Gibbs Energy. Relationships between thermodynamic properties. Residual properties. Biphasic systems. Generalized correlations.

4.- Thermochemistry

Determination of heat capacity. Methods of calculation of heat of phase change. Entalpies of formation. Reaction Enthalpy.

5.- Variable composition systems: Estimation of mixing properties

Estimation of volumetric properties of mixtures. Mixing rules. 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. Models for its calculation.

7.- Chemical Equilibrium

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

Methodology

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.

Activities

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

Assessment

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 and 3/10 in each partial test to pass the subject per 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

Assessment Activities

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

Bibliography

Koretsky, M.D. Engineering and Chemical Thermodynamics. John Wiley and Sons Ltd. USA. (2007)

Smith, J.M.; Van Ness, H.C. Introduction to Chemical Engineering Thermodynamics. 7th ed. McGraw-Hill Education. (2005).

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).