Chemical Thermodynamics

Calendar: 3rd day semester

Contact Hours: T 30,0h; TP 22,5h; OT 7,5h

Scientific Area: Chemistry

Intended learning outcomes (knowledge, skills and competences to be developed by the students):

The curricular unit has the main goal that student acquires knowledge and competences in the areas of applied thermodynamics to Petroleum Technologies.

It is essential that the students understand and predict physical properties of ideal and real gases, knowing how to apply the three laws of thermodynamics to reactions, allowing them to predict and calculate heat and/or work exchanges, entropy variations and spontaneity of the processes.

The student must be able to interpret phase diagram of pure substance, understanding the meaning of triple and critic points, and also to interpret different phase diagrams for mixtures, establishing the basis for several industrial separation process.

It is also necessary that student understand the differences between ideal and real liquid mixtures and the importance of the activity coefficients concept, allowing them to control the variables that affect the equilibrium.

Syllabus:

1. Brief review of some fundamental concepts of Physics.
2. Gases: Perfect gases. Kinetic theory of gases. Real gases – state equations (abreviated).
3. 1st thermodynamics law: Definitions. Work and heat. Internal energy and enthalpy.
4. Thermochemistry: Transitions enthalpies. Types of enthalpy. Temperature effect.
5. 2nd thermodynamics law: Entropy and the 2nd law. Absolute entropy and the 3rd law. Gibbs energy and spontaneity – properties.
6. Phase equilibrium: Transitions thermodynamics. Variation of the Gibbs energy with pressure and temperature. Phase diagrams – interpretations and examples. Liquids molecular structure.

7. Mixtures: Introduction. Ideal solutions. Real solutions and activities. Colligative properties. Mixture phase diagrams – volatile and non-volatile liquids and solid-liquid.
8. Chemical equilibrium: Thermodynamics basis. Standard Gibbs energy. Equilibrium constant and composition. Le Chatelier's principle. Van't Hoff equation.

Evidence of the syllabus coherence with the curricular unit's intended learning outcomes:

The main goal of this UC is to allow the student to acquire thermodynamics basic knowledge applied to Oil and Gas Engineering.

The 2nd chapter refers to the gases properties and is essential for homogeneous and heterogeneous system control, either in ideal or real conditions, involving gas phase.

Chapters 3, 4 and 5 are referent to thermodynamics laws and thermochemistry, are fundamentals for energy flow studies, especially heat exchanges, which are essential to study heat exchangers, furnaces, cooling towers, etc.

In chapters 6 and 7 are referent to the study of phase diagrams and ideal and real solutions. These are very important subjects to processes control that include phase change, such as distillation towers, vaporizers, etc., and for general processes which usually involve formation of precipitates and solutions.

Finally, chapter 8 refers to equilibrium which is essential for reactors processes, in which such phenomenon can be used as system control.

References:

1. Physical Chemistry, Peter Atkins and Julio de Paula, OUP Oxford; 9th edition, ISBN-10: 0199543372, 2009

2. Elements of Physical Chemistry: Peter Atkins and Julio de Paula, OUP Oxford; 5th edition, ISBN-10: 0199226725, 2009

3. Termodinâmica Aplicada, Edmundo Gomes de Azevedo, 3ª Edição, Escolar Editora, ISBN-10: 9789725923153, 2011

4. Introduction to Modern Thermodynamics, Dilip Kondepudi, John Wiley & Sons, ISBN-10: 0470015993, 2008

5. Thermodynamics (SI units): An Engineering Approach, Yunus A. Cengel and Boldes, McGraw-Hill Higher Education; 6th edition, ISBN-10: 0071257713, 2007

6. Engineering Thermodynamics: Work and Heat Transfer, Gordon Rogers and Yon Mayhew, Longman Scientific; 4th edition, ISBN-10: 0582045665, 1992