# uc3m Universidad Carlos III de Madrid

## Chemical basis of engineering

Academic Year: ( 2022 / 2023 ) Review date: 31-05-2022

Department assigned to the subject: Materials Science and Engineering and Chemical Engineering Department

Coordinating teacher: POZUELO DE DIEGO, JAVIER

Type: Basic Core ECTS Credits: 6.0

Year: 1 Semester: 1

Branch of knowledge: Engineering and Architecture

#### **OBJECTIVES**

By the end of this content area, students will be able to have:

- 1. Knowledge and understanding of the chemical basis, organic and inorganic applied chemistry underlying the branch of industrial engineering;
- 2. The ability to apply their knowledge and understanding to identify, formulate and solve problems of chemical basis, organic and inorganic applied chemistry using established methods;
- 3. The ability to design and conduct appropriate experiments of chemistry, interpret the data and draw conclusions;
- 4. Workshop and laboratory skills in chemistry.
- 5. The ability to select and use appropriate equipment, tools and methods to solve problems of chemical basis, organic and inorganic applied chemistry;
- 6. The ability to combine theory and practice to solve of chemical basis, organic and inorganic applied chemistry.
- 7. The ability to function effectively both individually and as a team.

#### **DESCRIPTION OF CONTENTS: PROGRAMME**

Topic 01.- The atom and its periodic properties

- Introduction. Electromagnetic radiation. Wave-particle duality. Bohr's atomic model. Concept of probability. Schrodinger approximation.
- Atomic orbitals. Energy of orbitals. Order of filling atomic orbitals. Exceptions to the filling rule. Electronic configuration in monoatomic ions.
- Periodic properties Atomic radii Ionic radius Ionisation energy Electronic affinity Electronegativity.

#### Topic 02.- Chemical Bonding

- Ionic bonding. Crystalline structure. Properties of Ionic Compounds.
- The Covalent Bond. Ionic character of the covalent bond. Polarity of molecules. Valence bond theory. Hybridisation.
- Metallic bonding. Structure of the metallic bond.
- Intermolecular forces.

## Topic 03.- States of Matter. Gases, Liquids and Solids.

- Gases. Kinetic theory of gases. Mixtures of Ideal Gases:
- Changes of state. Vapour-liquid equilibrium. Variation of vapour pressure with temperature.

Clausius equation. Clausius-Clapeyron equation.

- Phase diagram.

# Topic 04.- Dissolutions and Colligative Properties.

- Introduction. Ways of expressing concentration.
- Solubility. Factors that influence solubility. Solubility of gases. Henry's law. Partition law.
- Ideal gas solubility. Raoult's law Deviations from Raoult's law.
- Boiling point diagrams. Distillation Freezing point diagrams

- Colligative properties Decrease in vapour pressure. Increase in boiling temperature. Decrease in melting/freezing temperature. Osmotic pressure.

## Topic 05.- Thermochemistry

- Definition of Thermochemistry and Types of Systems
- State Functions
- Heat, Enthalpy and Heat Capacity.
- Enthalpy and chemical reactions.
- Indirect determination of enthalpies: Hess' Law
- The first principle of thermodynamics: Heat, Work and Enthalpy.
- The second principle of thermodynamics: Entropy and disorder, Spontaneity, reversibility and equilibrium.
- Absolute Entropy and the third principle
- Free energy and spontaneity

## Topic 06.- Chemical equilibrium.

- Reversible reactions.
- Equilibrium constants.
- Homogeneous equilibria.
- Heterogeneous equilibria.
- Factors affecting chemical equilibrium.

## Topic 07.- Acid-base equilibria and solubility.

- Acid-base definitions. Arrhenius theory. Bronsted-Lowry theory. Lewis theory.
- Acid-base properties of water. Acid, basic and neutral solutions.
- Strength of acids and bases Relationship between acidity constant and basicity constant.
- Hvdrolvsis.
- Common ion effect. Buffer solutions
- Solubility Solubility product Precipitation reactions Effect of common ion on solubility.
- Industrial examples.

#### Topic 08- Electrochemistry.

- Concept of Oxidation and Reduction.
- Types of Batteries.
- Applications of galvanic cells.
- Applications of electrolytic cells. Faraday's Law.
- Potentials of Redox Processes.
- Spontaneity of Redox Processes.
- Effect of Concentration on Potential.
- Corrosion stacks Cathodic protection and passivation.

# Topic 09.- Chemical Kinetics.

- Reaction rate.
- Rate laws and reaction order
- Arrhenius Law
- Reaction mechanisms
- Homogeneous and heterogeneous catalysis
- Chemical reactors

# Topic 10.- Introduction to Chemical Engineering

- Concept and fundamentals of Chemical Engineering.
- Transport phenomena.
- Balances of matter.
- Main basic physical operations.

# Topic 11.- Introduction to Organic Chemistry.

- Identification of the families of organic compounds. Nomenclature of organic compounds.
- Hydrocarbons. Description of the bond in saturated and unsaturated hydrocarbons.

## Nomenclature and formulation of hydrocarbons. Physical properties of aliphatic hydrocarbons

- Types of organic reactions. Reaction intermediates: radical, carbocation and carbanion. Aliphatic and aromatic hydrocarbons.

- Main sources of hydrocarbons: petroleum, natural gas and coal.
- Petroleum processing Industrial use of fossil fuels

- Alcohols, phenols and ethers. Properties, methods of production. Applications
- Aldehydes and ketones. Properties, reactivity.
- Organic acids. Properties, reactivity. Polymerisation.

#### LEARNING ACTIVITIES AND METHODOLOGY

Master classes, tutorial classes in small groups dedicated to resolving student questions and doubts, student presentations, individual tutorials, and individual work by the students; activities dedicated to acquisition of theoretical knowledge related to the lecture course (3 ECTS credits)

Laboratory practical sessions and classes in small groups dedicated to solving question sheets, individual tutorials and individual work by the student; activities dedicated to acquisition of practical skills related to the lecture course (3 ECTS credits)

#### ASSESSMENT SYSTEM

% end-of-term-examination: 55
% of continuous assessment (assignments, laboratory, practicals...): 45

Continuous assessment (45%):

- There will be three 50-minute tests in small groups.
- 1st test: Topics 1-4 (10% of the mark); 2nd test: Topics 5-8 (10% of the mark); 3rd test: Topics 9-11 (10% of the mark).
- A paper on industrial processes will be required (5% of the mark).
- Participation and handing in a report of the practical laboratory sessions (10% of the final mark).

Laboratory practices are mandatory for being assessed.

Final exam (55%).

#### **BASIC BIBLIOGRAPHY**

- K. HEINZ BÜCHNER, HANS-HEINRICH MORETTO, P. WODITSCH, Industrial Inorganic Chemistry, Wiley-VCH; 2000..
- K. WEISSERMEL, HANS-JÜRGEN ARPE, Industrial Organic Chemistry, 4th Edition, Wiley & Sons; 1997...
- P.W. ATKINS, L. JONES. Chemical Principles, W H Freeman & Co, 2001.
- R. CHANG. Chemistry,, McGraw-Hill Science, 2006..
- RICHARD M. FELDER, DONALD W. ROUSSEAU Elementary Principles of Chemical Processes, John Wiley & Sons.