NATIONAL UNIVERSITY OF ENGINEERING
COLLEGE OF SCIENCES
CHEMISTRY PROGRAM

CQ063 – CHEMICAL CATALYSIS

I. GENERAL INFORMATION

CODE	**:**	CQ063 – Chemical Catalysis
SEMESTER	**:**	9 - 10
CREDITS	**:**	06
HOURS PER WEEK	**:**	08 (Theory – Practice – Laboratory)
PREREQUISITES	**:**	CQ252 Physical-chemistry II
CONDITION	**:**	Elective

II. COURSE DESCRIPTION

The main objective of this course is to familiarize students with the fundamental concepts of heterogeneous catalysis, based on concepts of Inorganic Chemistry (heterogeneous catalysts are inorganic materials), Physical Chemistry, Chemical Engineering and Materials Science. This subject is divided into two parts: the first describes the general principles of heterogeneous catalysis and the second gives the most important industrial applications.

III. COURSE OUTCOMES

By the end this course the student will:

- Represent adsorption and catalysis in terms of energy exchanges and obtain from the textural analysis of the catalyst, the type of porosity, the surface magnitude and the pore size distribution.
- Characterize the influence of geometric and electronic factors on the catalytic action.
- Organize the structural, chemical, textural information of the catalytic materials from surface and mass characterization techniques and their relationship with the activity and selectivity of the catalysts.
- Research and design catalysts based on metal oxides to eliminate volatile compounds in work environments.
- Project simple kinetic expressions for heterogeneous reactions catalyzed according to the controlling stage.
- Develop a basic kinetic based on the SCIENTIST program to obtain the most suitable kinetic model.

IV. LEARNING UNITS

1. **Introduction / 4 HOURS.**
   Introduction / Fundamental concepts / Catalysis objective / History and relevant catalytic innovations / Stages of a catalytic process / Classification of catalysis / Concepts applied to catalyst activity / Types of catalytic processes / Relationship: Preparation-Characterization-Activity / Relevant characteristics of a catalyst / Catalytic reaction vs stoichiometric reaction.

2. **Physisorption / 6HORAS.**
   Application of the physisorption techniques to the textural study of solids / Determination of the specific surface of porous solids / Classification of the isotherms of adsorption / Types of porosity / Distribution of pores sizes / Other techniques for the textural study of solids / Application examples .

3. **Chemisorption / 6HORAS.**
   Chemisorption: Its application in the chemical characterization of solid surfaces / Particular study of some chemical adsorption processes on metals and metal oxides / Techniques for the experimental study of chemisorption phenomena / Examples of application.

4. **Heterogeneous catalysts / 6HORAS.**
   Heterogeneous catalysts / Design criteria for heterogeneous catalysts / Fundamental constituents of a heterogeneous catalyst: active phase, promoter and support / General methods of catalysts preparation / Active site / Structurally sensitive reactions / Gas-solid reactions / Transport phenomena: internal and external diffusion / Influence of transport phenomena on catalytic activity / Application examples.

5. **Characterization of heterogeneous catalysts / 6HORAS.**
   Characterization of heterogeneous catalysts / Set properties / Surface properties. Particle properties: mechanical, textural, density, size, fluid-mechanical / Density properties. Characterization techniques: surface (XPS, SEM-EDX), volumetric (XRD, TGA, TPR) / Application of gas chromatography in the catalytic analysis / Application examples.

6. **Metal catalysts / 6 HOURS.**
   Supported metal catalysts / Deposition techniques of the metallic phase. Common methods of activation / Chemical and nano-structural characterization of supported metal catalysts / Metallic dispersion concept and its experimental determination / Application examples.

7. **Main catalytic materials / 6HORAS.**
   Main catalytic materials: metals, metal oxides / Catalytic supports: silica, alumina, titania. Metal-support interactions. Metal oxides: supported and not supported / Zeolites. Perovskitas / Stacked clays (PILC`s) / Metallic catalysts / Examples of application.

8. **Notion of catalytic reactors / 6HORAS.**
   Notion of catalytic reactors. General / Classification of reactors / Batch reactors, stirred tank, continuous / Piston flow reactors / Elemental equations of material and energy balances. Reaction rate applied to batch and continuous reactors / Concept of spatial velocity and time / Membrane reactors, advantages of their application / Examples of activity measurement, selectivity and performance.

9. **Notion of kinetic modeling / 6 HOURS.**
   Notion of kinetic modeling / Non-mechanistic models (potential model) and mechanistic models: Mars-Van Krevelen model / Langmuir-Hinshelwood model / Discrimination of kinetic models / Statistical parameters of discrimination: MSC (model selection criterion) / DC (determination coefficient). Correlation coefficient / Application of the SCIENTIST program for multivariate adjustment of kinetic data. Data convergence / Examples of application in COV's combustion reactions.

10. Reactions of industrial importance / 4 HOURS.

Industrial importance reactions / Hydrogenation reactions / Importance and applications / Catalytic combustion reactions / Importance in the chemical industry / Environmental applications of heterogeneous catalysis / Catalysts for VOC's elimination (volatile organic compounds) / TWC catalysts ("Three Way" Catalysts ") to control the pollution generated by the exhaust gases of automobiles. Application examples.

V. LABORATORIES AND PRACTICAL EXPERIENCES

Laboratory 1: Determination of the BET surface of carbonblack by single-point multipoint methods. Description of the GEMINI VII physisorption equipment.

1st Qualified practice.

Laboratory 2: Evaluation of the pore size of an oxide sample by the Halsey and Hankins-Jura method.

Laboratory 3: Preparation of heterogeneous mass catalysts based on metal oxides.

2nd Qualified practice.

Laboratory 4: Preparation of supported heterogeneous catalysts based on metal oxides.

Laboratory 5: Characterization of catalysts by the TPR technique. Equipment: chemisorb 2720.

3rd Qualified practice.

Laboratory 6: Characterization of catalysts by the TPD-O2 technique. Equipment: chemisorb 2720.

Laboratory 7: Characterization of catalysts by the FTIR technique.

4th Qualified practice.

Laboratory 8: Reaction of oxidative dehydrogenation of ethane. W/F concept. Measurement of the activity.

VI. METHODOLOGY

The methodology is based on the exposition of the theoretical material, using the audio-visual materials available (slides and transparencies), providing the student with the necessary material for the good follow-up of the course. The course pursues the active interaction of the student to ensure the understanding of the concepts developed in the course.

VII. EVALUATION FORMULA

Final grade calculation: PE (weight 1) + FE (weight 1) + Practices average (weight 1) / 3
PE: Partial Exam – FE: Final Exam

Note: The practices are carried out in the Physical-Chemistry Research Laboratory - LABINFIS (R2-409).

VIII. BIBLIOGRAPHY

- Augustine Robert, Heterogeneous Catalysis for the Synthetic Chemist, Marcel Dekker Inc. New York, 1996.
- Hegedus L., Catalysis Design, John Wiley and Sons, New York 1987.
- Jones A., Mcnicol B., Temperature Programmed Reduction for Solid Materials and Characterization, Chemical Industries/24.
- Somorjai G. A., Introduction to Surface Chemistry And Catalysis, John Wiley & Sons (1994).
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- Fogler H.S. Elements of Chemical Reaction Engineering, 3ª Edición. Ed. Prentice-Hall International, Inc. New Jersey (1999).

- Farrauto R.J., Bartholomew C.H., Fundamentals of Industrial Catalytic Processes, U.S.A. 1997.

- Bond G. C., Heterogeneous Catalysis. Principles and Applications. Oxford, University Press (1987).

- Heck R.M., Catalytic Air Pollution Control, Commercial Technology (2ª Ed).

- Journals in Catalysis: Journal of Catalysis, Applied Catalysis, Journal of Molecular Catalysis, Chemical Engineering, Journal, Http://Www.Sciencedirect.Com/Science/Journal/15726657.