

## COURSE SYLLABUS

### 1. Identification

Code and title: QUP 018 - Homogeneous and Heterogeneous Catalysis

Professor: Michèle Oberson de Souza, Kátia Bernardo-Gusmão and José Ribeiro Gregório

Level: Master and Doctorate

Credit hours: 3

Revised: August\_2019

### 2. Summary

Homogeneous catalysis. Reaction quantities. Coordination and organometallic chemistry in catalytic processes. Main classes of processes in homogeneous catalysis. Industrial processes in homogeneous catalysis. Heterogeneous catalysis. Adsorption phenomena. Solid supports, surface modification of supports with organic groups, metals, oxides and complexes. Characterization methods. Main industrial processes in heterogeneous catalysis. Ziegler-Natta Catalysis. Study of molecular and surface catalytic systems: synthesis, characterization, properties and applications of homogeneous and heterogeneous catalytic precursors.

### 3. Objective

The course aims to present / discuss homogeneous and heterogeneous catalytic systems of academic and industrial interest.

### 4. Contents

- General Concepts in Catalysis. Catalysts, cocatalysts, promoters and modifiers. Reaction, Conversion, Selectivity, Yield, Activity, Turnover Number, Turnover Frequency, etc. Catalytic reaction kinetics. Catalytic cycles: main characteristics in homogeneous and heterogeneous systems.
- Homogeneous Catalysis. Coordination chemistry and organometallic applied in catalytic systems. Catalytic reaction mechanisms involving transition metal complexes. Catalytic processes. Isomerization. Hydrogenation. Oligomerization. Polymerization. Metathesis. Hydroformylation. Carbonylation. Oxidation. Coupling Reactions. Asymmetric catalysis: main concepts. Industrial processes: Wacker, Shop, Dimersol, Monsanto, DuPont, Reppe, etc. Industrial processes in fine chemistry: Heck, asymmetric hydrogenation, Sharpless epoxidation, cyclopropanation, etc. Homogeneous Ziegler-Natta.
- Heterogeneous Catalysis. General concepts in heterogeneous catalysis (comparative table between homogeneous and heterogeneous catalysis). Organic and inorganic supports: preparation, properties, activation, functionalization, etc. Preparation of heterogeneous catalysts: methods of impregnation, ion exchange, precipitation, vaporization, grafting, etc. Industrial methods: spraying, pelleting, etc. Zeolites: classification, properties, applications, ... Analysis techniques: spectroscopic methods (FT-IR, CP-MAS, NMR, SEM, XPS, etc.), thermal methods (TPD, TPR, TPO), volumetric methods (BET, porosity measures, etc.). Catalytic processes: hydrogenation, hydroformylation, oxidation, reduction, methanation, etc. Main industrial processes: hydrocarbon reforming, Fischer-Tropsch, MTG process, Ziegler-Natta, pollution catalysts.

## 5. Assessment

Written evaluation will be performed with the contents of homogeneous catalysis and heterogeneous catalysis. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:

- A: grade equal to or above 9.0
- B: grade equal to or above 7.5 and below 9.0
- C: grade equal to or above 5.0 and below 7.5
- D: grade below 5
- FF: lack of frequency

## 6. Methodology

Lectures, exercises lists, seminars and examinations.

## 7. Bibliography

- G. W. Parshall and S. D. Ittel, Homogeneous catalysis, Wiley, Nova Iorque, 1992.
- C. Masters, Homogeneous Transition-Metal Catalysis: A Gentle Art, Chapman and Hall, Nova Iorque, 1981.
- B. Frémaux, Éléments de Cinétique et de catalyse, Technique et Documentation, Paris, 1989.
- G. Henrici-Olivé and S. Olivé, Coordination and Catalysis, VCH, Heidelberg, 1977.
- H. Brunner and Z. Zettlmeir, Handbook of Enantioselective Catalysis with Transition Metal Compounds, VCH, Nova Iorque, 1993.
- R. Noyori, Asymmetric catalysis in Organic Syntheses, Wiley, Nova Iorque, 1993.
- K. Weissmehl and J. H. Arpe, Chimie Organique Industrielle, Masson, Paris, 1981.
- R. B. Anderson and D. T. Dawson, Experimental Methods in Catalytic Research, vol. 1 a 3, Academic Press, Londres, 1976. - Artigos recentes de revistas especializadas.