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Graduate Program in Chemistry (Grade 7/CAPES)
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COURSE SYLLABUS

1. Identification

Code and title: QUP403 - CO_2 Chemistry - Technologies and New Materials
Professor: Maria do Carmo Rangel, Kátia Bernardo-Gusmão and Michèle Oberson de Souza
Level: Master and Doctorate
Credit hours: 3
Revised: February_2021

2. Summary

Environmental impact. Energy generation processes. Physicochemical properties and CO2 capture. Use of CO2 for advanced oil recovery. Catalytic production of CO and synthesis gas. Photochemical production of hydrogen. Sustainable carbon economy. Catalytic processes for obtaining fuels. Comparison between technologies and perspectives for the future.

3. Objective

Familiarize the student with new technologies and materials related to the capture and storage and/or use of carbon dioxide, in the context of environmentally correct policies and green processes.

4. Contents

4.1 Environmental impacts of carbon dioxide emissions. Carbon dioxide emitting sources: means of transport; energy generation processes (pre-combustion and combustion) and petrochemical and petroleum refining processes (FCC, naphtha reforming; natural gas reforming, catalytic production of CO and synthesis gas (use of metallic oxides); WGS (water gas shift), post-combustion; oxy-combustion and other industrial processes). Properties of carbon dioxide molecules and their action in depleting the ozone layer and global warming. Need to capture atmospheric carbon dioxide.
4.2 Physicochemical properties and CO_2 capture. Phase diagrams; binary equilibria; solubility; absorption; adsorption/desorption; separation (membranes; porous materials, chemical and physical solvents).
4.3 Carbon capture and storage. Available technologies. Cryogenics. Comparison between technologies and perspectives for the future.
4.4 Sustainable carbon economy. Use of CO_2 for advanced oil recovery. Catalytic processes for obtaining fuels: catalytic production of CO (electrochemical or photochemical reduction).
4.5 Catalytic processes for obtaining chemical products using carbon dioxide. Production of hydrocarbons and olefins: Fischer-Tropsch, methanol, dimethylether, methane, alcohols and polyols. Dehydrogenation of alkanes and alkyl aromatics; reforming natural gas and hydrocarbons using carbon dioxide. Conversion of CO_2 to higher value-added products: Cycloaddition in epoxides for the synthesis of cyclic carbonates and polycarbonates. CO_2 hydrogenation: obtaining formic acid and methanol. Obtaining olefins, carboxylic acids and carbamates.
4.6 Photochemical production of hydrogen (algae).

5. Assessment

List of exercises, presentation and discussion of scientific articles, theoretical tests and/or directed works. The final grade will be composed of the average of the evaluations of eventual works and seminars (40%) and the average of the evaluations (60%). 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

- Sang-Eon Park, Jong-San Chang, Kyu-Wan Lee. Carbon Dioxide Utilization for Global Sustainability. Elsevier.
- T. Inui, M. Anpo, K. Izui, S. Yanagida, T. Yamaguchi. Advances in Chemical Conversions for Mitigating Carbon Dioxide (Studies in Surface Science and Catalysis). Elsevier.
- Michele Aresta. Carbon Dioxide as Chemical Feedstock. Wiley. VCH.
- M. Phil. Inamuddin, Carbon Dioxide Utilization to Energy and Fuels. Springer.
- Colin Baird & Michael Cann. Environmental chemistry. 4th edition. W. H. Freeman and Company, New York, pp. 33-36.
- Periódico “Journal of CO2 utilization” (Elsevier) e outros periódicos relacionados ao tema.