

M2 internship in kinetic modelling

Duration: 5-7 month

Location: IRCELYON/CNRS (Villeurbanne)

Starting date: 1st quarter 2020

Grant : 570 euros/month

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IRCELYON: IRCELYON is the largest CNRS department devoted for fundamental and applied research in Catalysis in France. It offers state of the art facilities as well as cutting-edge tools for the characterization of solid catalysts and adsorbents. The work will be carried out in the group "Engineering" headed by Drs. David FARRUSSENG and Yves SCHURMANN

Background: Beyond the formulation of catalytic active phases, the design of the catalyst carrier also named catalyst support is key for ensuring catalytic effectiveness. When testing catalytic powders at small laboratory scale, internal mass transport limitation can be ignored. In opposite, for embodiments such as pellets or beads of millimeter size, major mass transport limitations of reactants/products may occur especially when the active phase is dispersed in microporous or mesoporous surface. Despite its industrial importance, the investigation of support transport properties are rarely addressed in the scientific community

In the group, we recently have started to investigate quantitative relationships between the porous structures of catalysts, including hierarchical porosity at grain and pellet scales, for diverse classes for materials including alumina, zeolites and MOFs.

Work description. He/she will have to carry out catalytic tests in gas phase or triphasic phase processes. Before hands, thermodynamic will be estimated in order to set relevant experimental conditions. Catalytic results will be analyzed and kinetic models will be investigated in order to estimate internal mass transport limitations. The structural characterization will be carried out by appropriate techniques (XRD, SEM, TEM, N₂ physisorption, X-ray tomography...). Catalytic bodies will be tested in specially designed cells available on site.

Educational value: The student will be trained in advanced catalytic testing methods. Practical and theoretical aspects of Catalysis and Chemical Engineering are covered.

Candidates: Master in Chemical Engineering or in Catalysis with skills in modelling.

References:

Hollow Y zeolite single crystals: synthesis, characterization and activity in the hydroisomerization of n-hexadecane, C. Pagis et al, Oil & Gas Science and Technology, **2019**, 74, 38

Hydrogenation Size-Selective Pt/Hollow Beta Catalysts, AR. Prates et al, Chemistry- A European Journal, **2019**, 25(12) 2972-2977

Demonstration of Improved Effectiveness Factor of Catalysts Based on Hollow Single Crystal Zeolites, C. Pagis et al, CHEMCATCHEM, **2018**, 10(20) 4525-4529