NÉEL INSTITUTE Grenoble

Topic for Master 2 internship – Academic year 2020-2021

AI-assisted 3D image analysis of the microstructure of catalysts to reduce air pollution

General Scope:
The importance of catalysis is unequivocal in terms of economy, the impact on the quality of life, and in the fight against pollutant emissions. Additionally, catalyst is viewed as a key enabling technology, identified as one of the 12 principles of green chemistry. Progress in catalysis has always been motivated by societal needs, such as environment, energy, fuels, with the goal of improving the efficiency of the catalytic process on a technical scale. Technical catalysts are complex multicomponent bodies, ranging from dozens of μm to several cm, consisting of active phases, supports, and additives in shaped forms suitable for their application. They differ strongly from a research catalyst, i.e., the laboratory-developed materials constituted by a single bulk or supported active phase, which are the predominant focus of academic investigations. Yet despite tremendous relevance, understanding the complexity of these catalysts and their structure-property-function relationships has been largely neglected, mainly due to limitations of the characterization techniques. Ptychographic X-ray Computed Tomography (PXCT) is the 3D X-ray nanoimaging technique that overcomes these shortcomings. However, data post-processing to extract physical parameters out of the data is still challenging, but crucial for the optimization of these catalysts in oil-industry.

Research topic and facilities available:
This project comprises, among others, samples of Hydrodesulfurization (HDS) catalysts, and Fluid Catalytic Cracking (FCC) catalysts. Big data volumes obtained from the catalysts in synchrotron facilities will be available. This master project aims at the post-processing of 3D data for efficient quantitative characterization of the morphological structure and composition of the oil-industry technical catalysts using advanced 3D image processing tools and artificial intelligence. The outcome of this work will contribute to the manufacture of more efficient and less expensive catalysts. High-performance computing resources and adapted Python-based software will available for 3D image segmentation, assisted by deep-learning (E.g. UNet, DenseNet, FusionNet), to extract the required physical parameters out of the 3D image data.

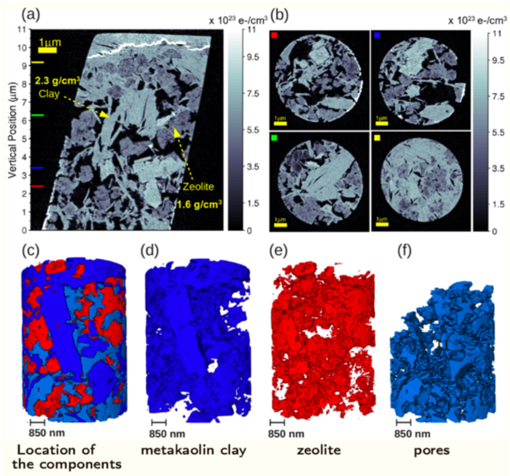

Figure 1 - (a-b) PXCT data obtained with FCC catalyst. (c-f) 3D image segmentation of the different catalyst material phases

Possible collaboration and networking:
The project will be carried out in collaboration including CNRS Institut Néel, French CRG beamlines at ESRF (FR), and KAUST catalysis center (KCC), Saudi Arabia. The 3D data will come from different synchrotron source facilities. Additionally, Grenoble is an important scientific hub hosting important research institution and technological companies

Possible extension as a PhD:
Depending on the intern performance and interest, there is a possible extension as a PhD if funding for a PhD thesis is obtained via a research project grant (already submitted) or Ph.D. contract award by the Physics Graduate School of University Grenoble Alpes.

Required skills:
Master in Physics, Chemistry, Materials sciences, Digital signal processing, or related domains. Scientific programming and/or image processing skills will be an asset.

Starting date: February 2021

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