PhD thesis offer within the BE-HyFE Project

Experimental study of catalysts and process designs for chemical synthesis using H_2 and CO_2

A 4-year position is currently available as a joint PhD between the Department of Chemical Engineering at the University of Liège and the Center for Sustainable Catalysis and Engineering of KU Leuven.

Context – BE-HyFE Project:

This PhD position is part of the Energy Transition Fund project BE-HyFE which aims to establish a core group of 16 broadly trained and highly networked early-stage researchers who can support the Belgian industry in finding both technological and societal solutions to essential hydrogen challenges. The project offers the selected candidate, next to an inspiring group dynamic with fellow researchers, a chance to establish specific hard and soft skills by means of a specialized training program (workshops, Hydrogen weeks, etc.), site visits to industry and (inter)national academic-industrial networking events. To encourage knowledge exchange and building the network, the present PhD research will be performed across two Belgian knowledge institutes, namely KU Leuven and University of Liège.

The specific topic of the present research addresses the reaction of hydrogen with CO_2. Indeed, CO_2 from industrial processes (short to middle term) or from the air (middle to long term) appears as a valuable resource to replace fossil-based materials in future industries. However, carbon dioxide is difficult to react due to thermodynamic considerations and also due to the high activation energies that are needed. Reactions with hydrogen offer a way out, since the energy is carried in the molecule. Combining hydrogen from renewable (the so-called power-to-X approach) with Carbon Capture and Use (CCU) has the advantage that it can produce synthetic methane, liquid fuels and other high value chemicals as a sustainable alternative to fossil-based fuels and chemicals.

Research objectives:

The goal of the present thesis proposal is two-fold: (i) to develop hybrid solid catalysts where CO_2 activation with H_2 happens on a reducible oxide surface, and (ii) to experimentally study such catalysts that react CO_2 and H_2 to synthesize added value bulk chemicals such as methanol, olefins, dimethylether, kerosene or other Fischer-Tropsch fuels. The ultimate goal of this research is to tackle the challenges associated with a whole range of reactions that were historically based on syngas (CO and H_2) and that now want to use CO_2 instead, contributing to the circularity of carbon and its removal from the atmosphere.

Methodology:

The present research will combine catalyst design, synthesis and optimization at KU Leuven with process design at ULiège. At KUL, the focus in catalyst development will be on integrating oxides capable of chemistry with oxygen vacancies and surface redox cycles (indium-zirconium, zinc…) with microporous zeolites to steer the hydrocarbon product distribution. The study will include several steps, among which catalyst synthesis and kinetic testing.

At ULiège, the study will consist in developing an experimental reaction set-up considering an available 6.6 kW alkaline electrolyzer. The work will be conducted in collaboration with on-going research focusing on Fischer-Tropsch synthesis. The reaction set-up will be designed in a flexible and modular way to allow CO_2 hydrogenation reactions at different operating conditions (temperature, pressure, feed gas composition…). Different catalysts will be tested: commercial references if available, as well as catalysts developed in the above-described steps. Focus will be set on the understanding of mass and heat transfer effects in order to identify control mechanisms and optimize reactor and process design. Analytic methods for characterization of the synthesized products will also be developed. The lab bench would be of an intermediate scale, leading to product synthesis in the range of 1-2 kg per day, enough to provide relevant data for process design and simulation.

The PhD thesis job also includes participation to project meeting, presentation of results at national and international conferences, writing of scientific articles... Collaboration and exchanges (including research stays) with national and foreign universities are also encouraged. The successful candidate will receive a PhD student position for a 4-year period. The grant amount is in accordance with university standards.

Candidate's profile:

Candidates must have graduated (Master's degree) in Chemical Engineering or similar field (catalysis, chemistry, process engineering, …). They should have a strong interest in experimental work catalyst development, process modeling, analytic chemistry. Candidates should also be able to work in relative autonomy typical for PhD thesis, as well as to easily interact with academic partners. They should demonstrate ability to synthesize information from a literature review, and to use critical mind to evaluate possible solutions to a given problem. They should have a good understanding of thermodynamics, kinetics, and mass transfer issues. Ease to communicate in English (oral and written) is required, French and Dutch are additional assets.

Research environment:

The successful candidate will conduct research activities both at KU Leuven and at the University of Liège, located in Belgian cities that are well connected by train (~30 min ride).

The exact time sharing between the two laboratories will be defined jointly with the research advisors and also will depend on the progress.

At the University of Liège, the successful candidate will join a young and dynamic team within the Department of Chemical Engineering (DCE). The DCE employs about 60 people mostly active in the fields of process engineering and materials science. It performs experimental research activities, as well as studies the modeling and control of physico-chemical and biochemical processes. It targets the development and optimization of innovative materials and processes that are also sustainable and financially viable. The present research project will be conducted in an international-friendly environment, with about 20 different nationalities present in the DCE. The DCE is also an active member of the FRITCO$_2$T platform (Federation of researchers in innovative technologies for CO_2 transformation) at ULiège, and a founding member of the CO_2 Value Europe Association.

At KU Leuven, the Center for Sustainable Catalysis and Engineering (ca. 50 people) resides in the faculty of Bioengineering Sciences of KU Leuven. CSCE is developing novel heterogeneous catalytic processes seeking the selective conversion of alternative feedstock into chemicals and materials. CSCE is developing novel porous materials, catalytic technology as well as engineering concepts. In short, CSCE strategies aim at synthesis-structure-activity' relations for catalysts; process integration for selective catalytic reactions and synthesis-performance-degradation schemes for chemicals and polymers. The Dusselier lab in specific pursues research in 3 research lines at CSCE: Zeolite/oxide synthesis, CO_2 and CH_4 valorization via heterogeneous catalytic processes and biodegradable plastics.

More information about the host institutions:
www.chemeng.uliege.be
www.biw.kuleuven.be/m2s/csce and www.dusselier-lab.org

Recruitment process:
Applications containing CV, cover letter and possibly reference letter(s) should be gathered into a single pdf file and sent by e-mail to secretary.chemeng@uliege.be with in object the mention "Application ULiège-KUL PhD Be-HyFE".

Application deadline is September 30, 2021. Candidates selected from this first round will be invited for an interview during which they will be asked to briefly present a previous topic they worked on. Start of the PhD is flexible but should take place between November 2021 and March 2022.