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Post-Doctoral position:

"Innovative nanostructured **M**etal **O**rganic **F**rameworks/**C**arbon materials **c**omposite for post-combustion **C**O_2 **c**apture by adsorption**"**

Context:

The aim of the project is a proof of concept at TRL 4, in realistic conditions of flue gas, that Moving Bed Microwave Swing Adsorption (MBMSA) can be considered as potential CO_2 capture solution at long-term. The materials to be used in this process are nanostructured composite materials based on combination of Metal Organic Frameworks (MOFs) and carbon materials (carbon black, graphene oxide) composites, MOF/carbons. The main goals are to demonstrate that the solution is (i) an effective post-combustion CO_2 adsorption/desorption process with CO_2 enhanced capture and (ii) allow cost/time/energy reduction on desorption thanks to microwave heating regeneration processes.

This step is a key step between the concept and the industrial application to validate or not the possibility of scale up of the process.

Thus, the objectives of this research are:

(i) Green synthesis of the composites with high working capacity (at least 1-2 mmol/g at p = 0.15 bar of CO_2 at room temperature), high selectivity (> 30), good chemical, hydrothermal and mechanical stabilities, green synthesis and suitable electrical conductivity to absorb microwave.

(ii) Design and test of Moving Bed Thermal Swing Adsorption process using microwave heating to desorb CO_2: Moving Bed Microwave Swing Adsorption (MBMSA): more efficient CO_2 capture process with lower energy penalty in contrast to reference absorption/regeneration processes using amine solvent.

A list of MOFs has been selected as good candidates for post-combustion CO_2 capture based in particular on developments carried out in the H2020-MOF4AIR project (Metal Organic Frameworks for Carbon Dioxide Adsorption Processes in Power Production and Energy Intensive Industries - https://www.mof4air.eu/), coordinated by UMONS. Based on it, at least 4 MOFs were considered: MIL-160 (Al), MIL-120(Al), MIL-53-NH_2 (Al) and CALF-20.
In the first phase of the project, the above-mentioned MOFs and composites with graphene oxide (GO) were synthesized using the same GO content (5%) and different synthetic routes: *in situ* and *post-synthetic*. The composites were shaped using different binders for their use in a process. All composites were fully characterized by IR spectroscopy, powder X-ray diffraction, thermogravimetric analyses, nitrogen porosimetry and by SEM microscopy.

Area of the proposed research:

- Determination of adsorption performances on shaped materials. (i) Measurements of CO_2, N_2, O_2, H_2O adsorption isotherms on shaped materials already synthesized. The effect of the binder will be evaluated in terms of uptakes. Co-adsorption properties (CO_2 uptake in mixture and selectivity) will be determined under relevant conditions (gas composition between 5% and 30% molar of CO_2 in N_2) by breakthrough curve measurements in a column of around 20 cm^3. Thanks to these measurements, mass transfer coefficients will also be determined. In addition, further crucial data relevant to the process (heat capacities and extensive cycling) will be measured or evaluated.

- CO_2 desorption by thermal heating and microwave heating. The desorption measurements will be achieved by thermal (hot gas), electrical and microwave heating on the different shaped materials. Different temperatures will be tested, depending on the ease of CO_2 desorption and the thermal stability to minimize the heating / cooling time and energy consumption.

- Effect of water upon CO_2 adsorption/desorption on shaped materials.

- Synthesis and shaping at the laboratory pilot scale. This task will consist in establishing optimized conditions to produce a few (2 or 3) shaped MOFs composites at the 400-500gram scale. The choice of the best samples will be carried out through the results from adsorption/desorption studies.

- Two or three shaped adsorbents will be tested in a lab-scale MSA reactor at room temperature with gas flowrates of 0.1 to 1 Nm^3/h of $CO_2/N_2/H_2O$. One will focus on finding the optimal conditions for adsorbent regeneration and gas recycling (GHSV, between 2000 and 10000 h^{-1}) giving the maximum process productivity still reaching the targeted CO_2 recovery and CO_2 purity of the product stream. Crucial points for the testing will be to determine the minimum temperature of regeneration, the mode of heating (continuous or pulse), and to study the heat transfer characteristics of the system and the adsorbents to further improvement. Energy consumption (MJ/kgCO_2captured) and productivity (kgCO_2 captured/(kg of adsorbent*h)) will be evaluated and compared to other processes.

The post-doctoral works will also naturally include different dissemination activities: reporting, scientific publications and presentations in international conferences.

During the works, several exchanges will be necessary with internal collaborators (PhD students, post-docs, etc.) and also with external collaborators such as other universities or research organisms, industrials, technology providers, etc.

Candidate's profile:

Education: Candidates must hold a PhD degree in Chemical engineering/Chemistry/Engineering Sciences or fields (such as industrial chemistry, mechanical/ environmental engineering, …) with a strong interest in chemistry, energy, environment, process engineering. Any previous experience in relation with carbon capture, especially by adsorption, would be an asset.

Languages: A good knowledge of English is required, both oral and written; a knowledge of French would be an asset.

Other skills: Any experience related to adsorption tests and adsorbent characterization would be an asset. Writing skills, good interpersonal and communication skills, rigor and conciseness will be highly appreciated.

The candidate will be hosted in a nice working environment under a challenging job at a dynamic and ambitious University, and in a context with several other PhD students/Post-docs working on carbon capture and utilization more particularly in the field of adsorption. Salaries are in accordance with the internal University agreement.

The Post-Doc is expected to start as soon as possible in 2024 for a duration until December 2025.

Recruitment procedure:

Applications (CV + motivation letter showing the adequacy with the requested profile + eventual letters of recommendation) should be sent by email to:

Prof. Guy DE WEIRELD:guy.deweireld@umons.ac.be ; +32 65/374203

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After a first selection based on the CV, the recruitment procedure will include minimum two interviews comprising a first remote interview by Microsoft Teams or phone, and a second interview (ideally in live at UMONS) including a short presentation by the candidate.