CHEMICAL ENGINEERING

MUR DM 117/Technip - Assessment of CO2 capture and conversion routes to valuable products in different applicative sectors

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Context of the research activity	The scope of this PhD is to evaluate different pathways for the conversion of captured CO2 to high added-value fuels and chemicals (i.e. syngas, methanol, DME, Aviation sustainable fuels, formate, alcohols, among others) with the aim to identify the most interesting ones, in terms of technical feasibility, environmental sustainability, potential improvement and future market needs. Electrocatalytic, thermocatalytic and biocatalytic technologies for converting CO2 containing flue gas streams will be analyzed with the final objective of developing the basic design of a pilot plant of the most promising selected process. Novel approaches of integrated CO2 capture and conversion processes, directly exploiting renewable-electricity will also be investigated. Progetto finanziato nell'ambito del PNRR - DM 117/2023 - CUP E14D23001980004

	CO2 is a key contributor to global climate change in the atmosphere. Its atmospheric level is increasing more than ever in the history of the Earth: It reached 419 ppm in January 2023 and will probably reach about 600 ppm by 2100, if the CO2 emission continues to follow the current trend. Currently, the European chemical industry strongly depends on carbon feedstock imports for energy and chemical manufacturing processes, which are based over 95% on the use of fossil fuels. Besides, the EU energy system is 80% based on fossil fuels that cause 80% of EU GHG emissions, and about 53% of the energy consumed in the EU is imported from outside countries. Exploiting sustainable chemistry, using renewable resources and CO2 to produce chemical products, brings an opportunity for efficient use of resources and preservation of the environment. It will contribute to reducing

Objectives	greenhouse gases, in line with the commitments agreed in the 2021 Glasgow Agreement signed during the United Nations Climate Change Conference (COP26). Carbon Capture and Utilization (CCU) is one of the major technologies that could be addressed worldwide to mitigate CO2 emissions. Currently exists different kinds of technologies that can be exploited to afford such challenge such as the electrocatalytic, thermocatalytic or biocatalytic CO2 hydrogenation processes, which are at different maturity levels and can be exploited for producing different target products. For instance, the electro-catalytic reduction of CO2 is a sustainable solution that can directly use renewable electricity (as source of electrons e-) and water (as a source of protons, H+) at ambient temperature to produce e-fuels of low carbon-based chemicals like Syngas (CO + H2), ethanol, ethylene, formic acid, among others. Instead, the thermocatalytic CO2 hydrogenation can exploit green hydrogen produced from water electrolysis for producing methanol, dimethylether (DME) or other fuels/chemicals at high temperatures (200-300oC) and pressure (up to 30bar). In this way, CO2 can be used as a feedstock in a circular economy perspective, transforming waste into useful and value-added products to tackle both GHG emissions and energetic problems related to the dependence on fossil fuels. This PhD will be divided into two main streams. The first one that will be developed in collaboration with Technip Energies, has the objective of defining the most promising routes for the CO2 conversion to valuable chemicals for specific applicative cases of study (e.g. cement, steel, petrochemical, chemical industries, among others) exploiting different assessment criteria such as techno-economic, environmental impact and current technology readiness level (TRL) of development. The second one aims to pursue the practical application of an integrated CO2 capture and conversion process already developed at Politecnico di Torino. The expected outcomes of the studies that will be performed in collaboration with Technip Energies are: • Investigation and classification of different CO2 conversion pathways (including electrochemical and thermochemical) in relation to different potential conversion products and their application sectors. • Detailed evaluation of selected technologies through process modelling of a specific applicative case of study, with the aim to elaborate a comparative techno-economic and environmental impact evaluation. • Selection of a pathway (relevant CO2 conversion process and target product) to be further studied in the following phases. The areas of improvement will be identified in terms of process performance looking to the selection of catalyst type and operating conditions. • The selected CO2 conversion technology will be validated at the laboratory scale by using the facilities available in the Politecnico di Torino under relevant environmental conditions, simulating real CO2 flue gas streams. The results will be correlated with the process performance for the future scale-up of the technology. • Based on the experimental results, a process model will be developed to be used for the fine tuning of the operating parameter to reach acceptable performance for further development. • Based on the laboratory tests and process simulation results, the most promising process scheme for CO2 utilization will be defined, including the required pre and posttreatment facilities, and the basic engineering design of a pilot plant will be developed in collaboration with Technip Energies. The expected outcomes of the studies that will be performed in the

	framework of previous knowledge of Politecnico di Torino are: • Optimization of an innovative process coupling CO_2 capture and in-situ electrochemical conversion. A reactor prototype developed between the Politecnico di Torino and an industrial partner within the European project SunCoChem (https://suncochem .eu/) will be exploited. The reactor operating conditions (flow rates, pressure, temperature, applied potential, etc) will be tuned to reach the target stability and electrochemical CO_2-to-fuels performance, under current density values (>100 mA/cm2) that are relevant for an industrial application. Different instruments available at PoliTO-DISAT and CREST Group https://www.disat.polito.it/it/la_ricerca/gruppi_di_ricerca/crest (e.g. Solar-Fuels Lab) and of the CO2 Circle Lab (https://co2circlelab.eu/) will be exploited for this research project.

Skills and competencies for the development of the activity	- Knowledge of chemical engineering and/or industrial chemistry is mandatory. - Experience with a process simulation software is required. - A good background or previous studies in catalytic processes or electrochemistry is highly recommended. - Good knowledge of standard practices and previous experience in chemical laboratories are desirable. - Ability to set priorities, work in a multicultural and multidisciplinary team, plan the work and respect deadlines are necessary. - Availability to work in lab or office in a full-time regime (8h a day x 5 days a week) is required.