POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 38th cycle

PNRR_352 Research Field: BIO-METHANE PRODUCTION FROM BIO-METHANATION OF RENEWABLE HYDROGEN: COMPUTATIONAL FLUID DYNAMICS (CFD) ASSISTED DESIGN OF BUBBLE COLUMN REACTORS EQUIPPED WITH MECHANICAL AND HYDRODYNAMIC AGITATORS

Monthly net income of PhDscholarship (max 36 months)
€ 1400.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	One of the main challenges faced by today¿s society is the increasing energy demand opposed to the need to curb environmental impact of human activities. In this context, **hydrogen from renewables** has been identified as a possible energy carrier, as it can be produced via electrolysis, stored, and later converted into energy in a variety of processes. Furthermore, the introduction of suitable energy carriers enables balancing loads on the network in scenarios where the share of solar, wind and tidal energy (inherently discontinuous sources) becomes widespread. Unfortunately, storage and transport of H_2 impose dedicated infrastructures and enhanced safety precautions, because of its high diffusivity and ample explosion limits. For these reasons, additional alternative energy carriers are being considered, such as CH_4 from H_2 and CO_2. This solution is compatible with the existing infrastructures and technologies for the storage and use of the gaseous carrier, providing, at the same time, alternative ways for reintroducing CO_2, that would otherwise be discharged in the atmosphere, in the energy cycle. The **bio-methanation** of renewable hydrogen and carbon dioxide is less energy demanding compared to thermochemical catalytic processes and better

	accommodates variable loads, an advantage when the energy supply is unsteady. Enabling the expansion of production of bio-methane well aligns with the targets defined by the European Commission¿s REPowerEU initiative, a recently introduced plan aimed at reducing dependence on foreign fossil fuels and fast-forwarding the **green transition** (https://ec.europa.eu/commission/presscorner/detail/en/IP_22_3131). These priorities are also coherent with the PNNR¿s mission supporting the green revolution, as it favors the integration of renewable energies in the existing national infrastructure system.The ultimate technical goal of this project is to develop industrial scale reactors for bio-methanation based on a novel technology by means of state-of-the-art simulations. The PhD candidate will interact with different academic and industrial national and international entities to gather the foundational knowledge for the simulations, to develop a physically sound computational model of the reaction units and to validate the numerical framework against pilot and large-scale reactors. The digital model will be a testing ground for different technological solutions, aimed at maximizing process yields at the industrial scale.
Methods and techniques that will be developed and used to carry out the research	The research project will focus on the **development of industrial technologies for the conversion of renewable hydrogen and CO_2 to bio-methane in a newly designed bioreactor**. The process will be based on a selected strain and reaction recently demonstrated on the bench/ pilot scale.Using modeling techniques describing the fundamental processes occurring in the bio -methanation process, the research will focus on the characterization of the mass and energy transfer phenomena controlling the reaction rate via **multiphase computational fluid dynamic (CFD)** simulations coupled with the reaction kinetics measured in lab-scale experiments. Experiments relevant to the biology of the process and transport phenomena of the gas/liquid system will be obtained through the collaboration with other academic institutions and partners, including the sponsoring company Pietro Fiorentini (PF) and MicroPyro, a start-up controlled by PF (collaborations are already in

	place). This experimental data will be incorporated in the multiphase reacting flow computations, supporting the identification of the most suitable models towards the accurate representation of the process. Meanwhile, PF will pursue the realization of pilot-scale and large-scale reactors towards the scaling up of the process. Direct comparisons between the computational results obtained from the simulations and the experimental results from small- and large-scale experiments will provide the validation for the modeling effort, guaranteeing that the numerical platform can provide a robust framework for the design and optimization of next generation bioreactors exploiting the same biological process. At this stage, the numerical model will offer insights into the potential of different mixing strategies in combination with a novel process and will clarify how they play in combination with different reactor geometries.The detailed CFD simulations will finally provide the basis for the calibration of simplified models useful to process simulation and optimization towards the definition of optimal operating regimes of the reactor within a complete hydrogen production and conversion plant. Finally, this project will offer opportunities for collaborations with entities and research institutions abroad. Among them, the student will have the possibility to collaborate with the research team located in Munich (Germany) who developed the proof of concept and the first bench-scale reactor for this novel process.
Educational objectives	By the end of this project, the PhD candidate will have developed the following skills: competence in computational fluid dynamics of reacting flows, chemical kinetics of biological systems, mass and energy transfer in multiphase systems, reactor and process design, processes for renewable energy carriers, industrial scale-up.
Job opportunities	By the end of this project, the PhD candidate will have gained skills relevant to multiple industrial sectors, including process engineering and design, pharmaceutical and bio-chemical processes, energy conversion and

	storage
Composition of the research group	2 Full Professors 2 Associated Professors 2 Assistant Professors 8 PhD Students
Name of the research directors	Prof.Marco Mehl

Contacts
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Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	700.0 €
By number of months	6

National Operational Program for Research and Innovation	
Company where the candidate will attend the stage (name and brief description)	Pietro Fiorentini S.p.A. Via Rosellini, 1 ¿ 20124 Milano Italy - HQ Via Enrico Fermi, 8/10 - 36057 Arcugnano (VI) https://www.fiorentini.com/
By number of months at the company	6
Institution or company where the candidate will spend the period abroad (name and brief description)	This project will offer opportunities for collaborations with entities and research institutions abroad, such as for example Munich (Germany). See the method section for further details.
By number of months abroad	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information

Confidentiality: since this is a thematic scholarship, the management of Confidential Information, Results and their publication is subordinate to the restrictions agreed upon with the funding company. Upon acceptance of the scholarship, the beneficiary must sign a specific commitment.

Individual budget for research (during the 3 years): about 5.400 euro

Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student. There are various forms of financial of for activities of support to the teaching practice. The PhD student is encouraged to take part in these activities within the limits allowed by the regulation.