



PhD in CHIMICA INDUSTRIALE E INGEGNERIA

CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 39th cycle

THEMATIC Research Field: GREENSOL - GREEN-BASED WATER-LEAN SOLVENT FOR CO₂ CAPTURE

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

Titolo: GREEN-based water-lean SOLvent for CO₂ capture

Acronimo: GREENSOL

CUP: D53D23003100001

Codice Progetto 2022774E9K

Decreto di Concessione: Decreto direttoriale di ammissione a finanziamento prot. n. 961 del 30 giugno 2023

In line with the mission of the Italian Government "Green Revolution and Ecological Transition", this research activity is configured as a Proof of Concept of a novel green-based water-lean solvent for application to the capture of CO₂, which is issued from anthropogenic emissions and strongly takes part in the adverse effects of global warming. The novel solvent, referred to as GREENSOL, will be composed of at least a bio-based component with the possible addition of other promoter(s) for CO₂ capture. The aim is to develop a novel environmentally-sustainable solvent able to efficiently remove carbon dioxide from gaseous streams with a reduction of the energy requirements for the regeneration section of at least 25%.

In detail, the main objectives (O) of the research are as follows:

O1: definition of the composition of GREENSOL;



	O2: measurements of CO₂ solubility, fluid phase equilibria and physical properties of GREENSOL; O3: development of a suitable thermodynamic model for GREENSOL in the Aspen Plus[®] commercial simulation software; O4: simulation of the CO₂ capture process in the Aspen Plus[®] commercial software; O5: techno-economic assessment of the CO₂ capture process using GREENSOL and comparison with the conventional process.
Methods and techniques that will be developed and used to carry out the research	The composition of GREENSOL will be defined using QSARs (Quantitative Structure-Activity Relationships) and Molecular Dynamics simulations in order to determine the best candidate in terms of CO₂ capture efficiency and health, safety and environmental impacts. Once the solvent composition has been established, the CO₂ capture process will be simulated for a flue gas reference stream in the Aspen Plus[®] commercial software. To this purpose, the most suitable thermodynamic property package will be selected and it will be properly calibrated, if needed, using the experimental data related to CO₂ solubility, fluid phase equilibria and physical properties, which will be collected during this research activity at the Process Thermodynamics laboratory (PT lab) of Politecnico di Milano. The resulting process simulation will be subject to a techno-economic analysis aimed at assessing the costs and energy requirements of the process for comparison with those of the conventional one. The aim of the proposed project is to find a green-based water-lean solvent for CO₂ capture that allows obtaining a reduction of the heat duty required for solvent regeneration of at least 25% compared to conventional solvents, while maintaining or improving the CO₂ capture efficiency. The outputs of the research will provide new expertise in the field of Carbon Capture Utilization and Storage (CCUS) and will also offer the possibility of enhancing the visibility of Italy as a promoter of cutting-edge research in that field.
Educational objectives	The planned research activity is expected to improve the



	capabilities and the knowledge of the PhD student in CCUS, so that he/she will then be able to design new sustainable processes.
Job opportunities	The expertise developed in the field of CCUS will favour the PhD student's career both in research centers and private companies that have been including CCUS strategies in their portfolio, as proved by the job started some months ago by a PhD student who is going to defend his thesis in one month.
Composition of the research group	1 Full Professors 1 Associated Professors 2 Assistant Professors 2 PhD Students
Name of the research directors	Prof. Moioli, Ing. De Guido

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

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
Educational activities (funding for participation in courses, summer schools, workshops and conferences) - financial aid per PhD student per year: 1st year: around 1.900 euros per student 2nd year: around 1.900 euros per student 3rd year: around 1.900 euros per student 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.