POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 40th cycle

THEMATIC Research Field: MODELING, SIMULATION AND REAL-TIME OPTIMIZATION OF DYNAMIC (BIO)CHEMICAL PROCESSES UNDER UNCERTAINTIES VIA WHITE AND BLACK BOX MODELLING

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	The main objective of this research will be the development of dedicated methodologies for the real-time optimization of (bio)chemical processes. In particular the focus will be on (bio)chemical processes for the biogas upgrading to bio-fuels and bio-chemicals (e.g., methanol, DME, SAF, etc). The research will focus on: 1) first principal, 2) data-driven black-box and 3) Generative AI methodologies. This will allow to identify the most interesting techniques for a specific scope, (i.e., simulation, dynamic optimization, optimal control). GenAI methodologies are emerging as powerful tools to perform ideation and language related tasks. This research will explore the possibility of applying and develop novel GenAI methodology for the modelling, optimization and control of (bio)chemical processes. This research is linked both to the Flexiby EU project and to the Swiss National research fund (SNRF). The Flexiby project focuses on the development of a novel process to convert algee into bio-fuels, while the SNRF is focused on the study of methanation and other (bio)chemical processes to upgrade biogas and bio-syngas to biofuels or biochemicals.
Methods and techniques that will be developed and used to carry out the research	This PhD research will focus on the development of the following methodologies and techniques:

	following methodologies and techniques: 1. Dynamic modeling and optimization package in python and o C++. The package will be based on first principal modelling methods and will allow the simulation of complex equipment?s such as reactors or separation units; 2. Non Linear optimal control and reinforcement learning package in python and or C++. This is an expansion of the previous package and will allow for the optimal control of complex (bio)chemical process. This package will include also online state and parameter estimation methodologies; 3. Development of Physics Informed Machine learning methodologies for the estimation and prediction of complex kinetic reaction parameters and integration of these method into first-principal models; 4. Development of an industrial modelling and physico-chemical parameter database for the most relevant (bio)chemical processes for the upgrade of bio material to biofuels or biochemicals; 5. Application and development of dedicated GenAI methods for the modelling, optimization and control of (bio)chemical processes.
Educational objectives	1. Advance knowledge in the field of dynamic modeling and optimization for (bio)chemical processes; 2. Advance knowledge in the field of optimal control for (bio)chemical processes; 3. Advance knowledge in the field of Physic Informed Machine Learning for (bio)chemical processes; 4. Advance knowledge in the field of biomass upgrading (bio)chemical process to fuels or chemicals; 5. Advance knowledge in the field of GenAI applied to the modelling, optimization and control of (bio)chemical processes

Job opportunities	•Co-founder for start-up emerging from PhD contribution •Post-Doc position in Italy or abroad •Industrial Data Analyst •Process/production engineer •Research Engineer
Composition of the research group	1 Full Professors 1 Associated Professors 1 Assistant Professors 0 PhD Students
Name of the research directors	Proff. Flavio Manenti, Mattia Vallerio

Contacts
Telephone: +39 3516846464 Email: mattia.vallerio@polimi.it Web-pages of the research group: https://super.chem.polimi.it/

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

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 will sign a specific commitment.

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:

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.