POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 39th cycle

PNRR 118 PA Research Field: MULTISCALE MODELING OF BIOMASS PYROLYSIS AND COMBUSTION

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	Biomass represent a renewable energy source and a viable substitute for fossil fuels. Thermochemical methods such as pyrolysis are employed to break down the complex structure of biomass into simpler molecular compounds. Biomass decomposition through pyrolysis is the first step also in other thermochemical processes such as gasification and combustion.The development of comprehensive chemical models plays a vital role in understanding biomass pyrolysis, gasification, and combustion. This complexity arises from the multicomponent, multiphase, and multiscale nature of biomass thermochemical conversion. Indeed, it involves various stages, starting from the accurate characterization of the feedstock, followed by the description of volatiles release at the particle level, and culminating in understanding the impact of secondary gas-phase oxidation or pyrolysis reactions at the reactor scale. All these aspects significantly influence biomass thermo-valorization processes and have a direct influence on valuable product distribution and on the formation of pollutants.The CRECK Modeling Lab has developed an advanced framework for modeling biomass pyrolysis and combustion. Widely regarded as the state-of-the-art in this field, this framework exhibits a remarkable capability to provide detailed compositions of pyrolysis and combustion products as well as solid residue (biochar).

	The objective of this doctoral program is to improve the model by undertaking the following activities:1. Characterize the composition of biomass by identifying key reference species such as cellulose, hemicellulose, lignins, extractives, proteins.2. Enhance the pyrolysis mechanism by incorporating the release of nitrogen-containing species (e.g., pyrrole) and their secondary gas-phase reactions, which play a crucial role in controlling the formation of NOx in combustion devices. Utilize newly available experimental speciation data to extend and refine the biomass kinetic model.3. Integrate the secondary (gas-phase) kinetic mechanism for biomass pyrolysis and combustion to explicitly account for particulate matter formation.4. Develop a reduced and optimized kinetic model for CFD simulations of biomass pyrolysis and combustion at the particle scale.5. Utilize the model to parametrically assess the impact of utilizing biomass in combustion devices, considering factors such as efficiency and emissions of pollutants (e.g., NOx, soot). Overall, this doctoral program advances the understanding of biomass pyrolysis and combustion at the fundamental level and supports the optimal design of biomass waste valorization processes for fuels, chemical and energy production.The proposed project is aligned with the topics and objectives of the National Recovery and Resilience Plan (PNRR), with particular reference to Agritech - National Research Centre for Agricultural Technologies (Spoke 8 – New models of circular economy in agriculture through waste valorization and recycling)
Methods and techniques that will be developed and used to carry out the research	The expertise available at the Creck Modeling Lab will enable the doctoral candidate to develop cross-cutting skills in kinetics and fluid dynamics aspects of biomass utilization. The candidate will investigate the chemistry of biomass thermal degradation (pyrolysis) and the role of the secondary gas-phase reactions in combustion. In particular, the formation of pollutants (NOx, soot) will be analyzed with a multi-scale approach, starting from elementary reaction pathways, up to the macroscale (i.e., combustors), where mixing and turbulence strongly interact with chemical kinetics aspects. The candidate will gain solid skills in biomass characterization and

	combustion simulations using detailed kinetics, including tools for kinetic mechanism reduction and optimization. In-house modeling tools will be available to the candidate (OpenSMOKE++, BioSMOKE++, DoctorSMOKE++, OptiSMOKE++, LaminarFOAM etc.).https://www.opensmokepp.polimi.it/ Furthermore, the candidate will include the data and kinetic models for biomass pyrolysis and combustion inside Sciexpem, a data ecosystem for experimental data and predictive models.https://sciexpem.polimi.it/ Innovhub-SSI has a consolidated experience in the investigation of pellet and wood stove combustors and the emission of polluting species. Over the past 20 years, Innovhub-SSI has determined and supplied the national competent bodies with the emission factors for domestic heating appliances and IC vehicles, which have been included in the national inventories of emissions. The main environmental issue, linked to the energy use of biomass, depends on the particulate matter produced by small domestic appliances, which represent over 90% of biomass consumption in Italy.The European regulation (EU Regulation 2015/1185) and the Italian legislation (DM 2017 n. 186) regulate and classify the appliances, that can be marketed and used at the European and national level, on the basis of their performances, in terms of efficiency and emissions (PM, CO, NOX, OGC). However, how to determine PM emissions and, consequently, what limits to impose is a very complex technical problem, that has engaged research centers, laboratories and regulatory bodies all over the world for decades, leading to the development of very different measurement methods, which produce very different results. The European reference technical standard (EN 16510-1:2022) has significantly changed the approach compared to the previous 2019 version. The basic problem lies in the presence of semi-volatile organic species, which can condense in the form of aerosols, adding to the primary solid component of the particulate matter (partly organic and partly inorganic). The extent of this phenomena can significantly shift the measured results, so that a deeper knowledge and modeling of the process can be very helpful in reconciling existing data.
Educational objectives	

	The primary educational goal of this doctoral program is to equip the PhD student with the necessary problem-solving skills to tackle a multi-scale and interdisciplinary problem and effectively address the involved research challenges. This problem encompasses various research areas, including i) feedstock/material characterization, ii) chemical kinetic and iii) Computational Fluid Dynamics (CFD) modeling.
Job opportunities	Job opportunities include R&D areas in the most varied industrial sectors, in particular those requiring advanced modeling skills. Straightforward areas include technology development (e.g. in energy and process industries), as well as opportunities in data science and process optimization fields.
Composition of the research group	2 Full Professors 2 Associated Professors 4 Assistant Professors 12 PhD Students
Name of the research directors	Prof. T. Faravelli /Prof. M. Pelucchi

Contacts
http://creckmodeling.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

National Operational Program for Research and Innovation	
Company where the candidate will attend the stage (name and brief description)	Innovhub-SSI - Via Giuseppe Colombo 83, 20133 Milano (https://www.innovhub-ssi.it)
By number of months at the company	6
Institution or company where the candidate will spend the period abroad (name and brief description)	da definire
By number of months abroad	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
The PhD student will have a dedicated pc and desk, and access to the Creck lab?s proprietary Linux High Performance Computing Cluster with ~700 processors located at POLIMI. Availability of in-house and commercial codes for CFD and combustion kinetic calculation (ideal reactors, kinetic mechanism reduction, flames, droplet combustion, solid particle pyrolysis-gasification-combustion, data management and analysis etc.) **Confidentiality**the management of Confidential Information, including results and their publication, associated to the activity with the company is subordinate to possible restrictions agreed upon with the company. Upon acceptance of the scholarship, the beneficiary must sign a specific commitment. **Individual budget for research** (5.700 euro):1st year: 1.900 euro; 2nd year: 1.900 euro; 3rd year: 1.900 euro **Teaching assistantship (availability of funding in recognition of supporting teaching activities by the PhD student):** there are various forms of financial 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.