



PhD in CHIMICA INDUSTRIALE E INGEGNERIA

CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 39th cycle

PNRR 118 INTERDISC Research Field: MODELING THE COMBUSTION CHEMISTRY OF HYDROGEN CARRIERS AND APPLICATION TO CARBON-NEUTRAL ENERGY CONCEPTS

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 use of energycarriers to store the excess energy produced byintrinsically discontinuous renewable sources (e.g., wind, photovoltaic) can be the key to a widespread decarbonization of processes for electricity production and transportation. For this purpose, the availability of kinetic models with predictivefeatures in different operating conditions is of primary importance,such that they can beapplied in the corresponding fluid dynamic(CFD) simulations of combustion processes (e.g., thermal engines). This doctoral program aims toperform the following activities:

1. Characterize the kinetic behavior of energy carriers (e.g. ammonia, dimethyl ether, methanol), both as pure compounds and in combination with each other and hydrogen.
2. Integrate the process knowledge obtainedat the previous stageinto a comprehensive and detailed kinetic model with validated predictive characteristics in the conditions of interest.
3. Develop a reduced kinetic model with a limited number of species for use in high-performance computing (HPC) simulations.
4. Evaluate the consequences in terms of efficiency and emissions of pollutants (NO_x , unburned



	<p>compounds) resulting from the use of these fuels in innovative energy processes.</p> <p>The proposed project is aligned with the topics and objectives of the National Recovery and Resilience Plan (PNRR), with particular reference to the components M2C2 "Renewable energy, hydrogen, grid and sustainable mobility"</p>
Methods and techniques that will be developed and used to carry out the research	<p>The expertise available within the two proposing research groups will enable the doctoral candidate to develop cross-cutting skills in kinetics and fluid dynamics with a strong applied focus, as already successfully accomplished in previous collaborations. In particular, the formation dynamics of polluting compounds will be analyzed with a multi-scale approach, starting from elementary reaction pathways, up to the macroscale (engine), where the role of turbulence in these processes will be examined. In addition to acquiring fundamental knowledge in quantum chemistry for reaction rate calculations and kinetic analysis, the candidate will gain solid skills in numerical methods, which will be utilized for kinetic mechanism reduction and subsequent optimization.</p>
Educational objectives	<p>The main educational objective of this doctoral program lies in providing the proper problem-solving skills to the PhD student such to face a multi-scale, eclectic problem, covering different but complementary research areas as i) theoretical chemistry, ii) chemical kinetic development and iii) CFD modeling.</p>
Job opportunities	<p>Job opportunities include R&D areas in the most varied industrial sectors, in particular those requiring consolidated modeling skills. Straightforward areas include technology development (e.g. in automotive and transportation engineering), as well as opportunities in data science and process optimization fields.</p>
Composition of the research group	<p>4 Full Professors 5 Associated Professors 4 Assistant Professors 14 PhD Students</p>
Name of the research directors	Prof. A. Stagni / Prof. G. D'Errico



Contacts
<p>http://creckmodeling.chem.polimi.it http://www.engines.polimi.it/</p>

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)	
By number of months at the company	0
Institution or company where the candidate will spend the period abroad (name and brief description)	Technische Universität Darmstadt - Otto-Berndt-Str. 2, 64287 Darmstadt, Germany - https://www.maschinenbau.tu-darmstadt.de/stfs/
By number of months abroad	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
<p>Individual budget for research (5.700 euro): 1st year: 1.900 euro; 2nd year: 1.900 euro; 3rd year: 1.900 euro</p> <p>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.</p>