POLITECNICO DI MILANO

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

PNRR 118 PNRR Research Field: DEVELOPMENT AND APPLICATION OF INNOVATIVE KINETIC ANALYSIS SYSTEMS

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 development of industrial processes of interest for the chemical industry as well as the investigation of the impact of products and materials used in the chemical industry on the environment requires a thorough understanding of the underlying reactive kinetics. This means that, in order to interpret such processes, a kinetic mechanism, either elementary or lumped, is necessary. This is often a limiting aspect in the development and optimization of traditional or new processes as the reaction kinetics is rarely known at the required level of detail. The consequence is that costly experimental campaigns are needed in order to gather the information necessary to build the kinetic mechanism. In this framework, the main aim of this project is the development of computational tools and protocols suitable to determine the reaction kinetics for systems whose reactivity is not well established. Three sectors of relevance for the PNRR objectives that are likely to benefit from the availability of these kinetic investigation tools and that will be the object of application of the approach developed in the PhD project are: •Climate change, in particular for what concerns the impact of new energy vectors (ammonia or hydrogen) on global warming (PNR area 5.5.1);

	•Environmental energetics, in particular for what concerns the use of new energy vectors (PNR area 5.5.2 and 5.5.4); •Industry 4.0 – digital transition, in particular for what concerns the development of digital twins of chemical reactors (PNR area 5.4.1);
Methods and techniques that will be developed and used to carry out the research	The methods and approaches that will be adopted in order to fulfill the aims of the project will consist in a synergistic use of computational fluid dynamic simulation and theoretical chemical kinetics methodologies, mostly relying on the use of the ab initio transition state theory based master equation approach. Kinetics simulations will be performed both using literature and home made software, in particular for what concerns the application of transition state theory to rate constant estimation. Most notably, automation and the exploitation of artificial intelligence algorithms will be included in the development of the simulation software. Fluid dynamic simulations will be performed using literature codes in order to determine temperature, velocity and composition fields relevant for the description of the systems of interest. The developed methodologies will be applied to the study of: •the use of hydrogen and ammonia as clean energy vectors, for example in fuel cells and in combustion engines; •the determination of the global warming potential of hydrogen accumulation in the atmosphere caused by leaking; •the development of digital twins for the synthesis of epitaxial silicon carbide (SiC) for power electronics applications. Relation to PNRRThe aims of the research are relevant to Mission 2 – Green revolution of the PNRR plan, and specifically M2C2 (Renewable energy, hydrogen, grid, and sustainable mobility) for what concerns the focus on hydrogen use and the estimation of its global warming potential (relevant to M2C2.3), and M1C2 (digitalization, innovation, and competitivity of the productive system), for

	innovation, and competitivity of the productive system), for what concerns investments in microelectronics. They are also in line with the PNR objectives, which are an integral part of the PNRR, as listed in the motivation section.
Educational objectives	Learn how to develop kinetic mechanisms suitable to describe complex reactive systems.Learn to use state of the art kinetic and fluid dynamic software.Learn how to apply the developed knowledge to optimizing systems of interest for the process industry.
Job opportunities	The PhD at the end of her/his pathway will have opportunities in different companies active in the process industry, either operating in the clean energy sector or in the microeletronic sector, in position of responsibility concerning not only research and development, but also process and product engineering.
Composition of the research group	5 Full Professors 3 Associated Professors 2 Assistant Professors 15 PhD Students
Name of the research directors	Prof. C. Cavallotti, Prof.ssa Busini

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)	
By number of months at the company	0
Institution or company where the candidate will spend the period abroad (name and brief description)	to be defined
By number of months abroad	6

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