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

THEMATIC Research Field: HYDROGEN IMPACT IN TERMS OF DISPERSIONS AND GWP

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	Modern economies focus on reducing GHG emissions to mitigate the effects of climate change. Countries around the world have begun to shift energy production by exploiting more and more renewable energy sources (RES). By 2040, EU RES-based technologies will account for 80% of new installed power, while, after 2030, wind energy is expected to become the main source of electricity. Wind energy, however, has problems associated with the variability of electricity generation, resulting from variable atmospheric conditions. To increase the application of RES, a significant development in energy storage technology is required in the electricity generation sector. Power-to-gas is an example of this technology: electrical energy can be converted into gaseous fuel (hydrogen). Hydrogen, as an energy carrier, can store the greatest quantities of energy and has a high energy content per unit of mass. Hydrogen has great importance as a promising green energy carrier, but it is not available in nature, thus it is usually generated as a secondary energy carrier from primary sources, such as natural gas or wind energy. When H2 is produced, transported, stored, and used, a part leaks into the atmosphere and the potential atmospheric impacts of increased emissions to the atmosphere of hydrogen have to be determined. Because Earth-system perturbation, which impacts tropospheric chemistry, creates a complex chain of events that alter the concentration of radiatively

	active atmospheric species (e.g., methane, ozone, and aerosols) a thorough understanding of the underlying reactive kinetics is necessary. This means that, 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 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. Once the kinetics is known, the dispersion of hydrogen from possible leaks has to be evaluated to assess primarily the flammable/explosive cloud that could form and then the contour of concentration of all the chemicals involved in the hydrogen reaction chain.
Methods and techniques that will be developed and used to carry out the research	atmospheric species (e.g., methane, ozone, and aerosols) a thorough understanding of the underlying reactive kinetics is necessary. This means that, 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 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. Once the kinetics is known, the dispersion of hydrogen from possible leaks has to be evaluated to assess primarily the flammable/explosive cloud that could form and then the contour of concentration of all the chemicals involved in the hydrogen reaction chain.

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 or in the microelectronic sector, in position of responsibility concerning research and development, safety, process and product engineering.
Composition of the research group	4 Full Professors 4 Associated Professors 3 Assistant Professors 15 PhD Students
Name of the research directors	Prof. V. Busini - Prof. C. Cavallotti

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.