POLITECNICO DI MILANO

PhD in CHIMICA INDUSTRIALE E INGEGNERIA CHIMICA / INDUSTRIAL CHEMISTRY AND CHEMICAL ENGINEERING - 37th cycle

PON - INNOVATION Research Field: NUMERICAL MODELING OF CHEMICAL VAPOR INFILTRATION "CVI" REACTORS FOR PRODUCTION OF CARBON DISK BRAKES FOR AIRCRAFT AND RACING APPLICATIONS

Monthly net income of PhDscholarship (max 36 months)
€ 1325.0 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	Chemical Vapor Infiltration (CVI) is the one of the leading techniques for the production of carbon disk brakes for aircrafts or high-performance vehicles. In CVI, highly porous preforms are placed in a reactor which is heated by surrounding electrical resistors. A gaseous medium (mainly composed of light paraffins) flows around the preforms and, thanks to the high temperatures, pyrolyzes. The decomposition products infiltrate the porous preforms, where heterogeneous reactions take place in the pores of the solid substrate, leading to the deposition of graphitic carbon.Currently adopted industrial CVI reactors present some important limitations. Their geometries do not promote homogeneous conditions (temperature and gaseous composition), with a negative impact on the final quality of carbon disks. In addition, the presence of undesired recirculation regions, leading to the formation of high molecular weight PAHs and soot, further decreases the performances of the process and complicates maintenance and cleaning operations. Moreover, in order to favor infiltration of decomposition products by diffusion and avoid formation of carbon crusts over the preform surface, the deposition rate has to be kept sufficiently slow, leading to a significant increase of time required for completing the densification (days).The present project aims at developing new, innovative reactor

	concepts (geometry and conduction of the operations), able to ensure a better densification process, with higher quality of the final carbon disks and reduced densification times. The activity will be carried out in collaboration with Brembo S.p.A., a world leader and internationally-recognized innovator of disc brake technology for automotive vehicles. During the research period abroad (in Nagoya University, Japan), the candidate will deepen the understanding of the densification process, through the combination of experimental measurements carried out on a lab-scale apparatus and detailed numerical simulations.More specifically, the objectives of the projects are the following: to develop and implement a numerical methodology to model the chemical vapor infiltration process in industrial scale reactors, by combining CFD (Computational Fluid Dynamics) and detailed homogeneous and heterogeneous chemistry; to develop a mathematical model to correlate the quality of deposited carbon to the local operating conditions to which single preforms are exposed; to explore the impact of alternative reactor geometries and unconventional operating conditions (ie oscillating pressure) on the densification process and the quality of the final product; to develop a digital twin of a CVI reactor for industrial production available in Brembo.The objectives reported above are in line with the "Innovative, highly efficient production processes for industrial sustainability¿ development trajectory in National Smart Specialisation Strategy (NSSS)".
Methods and techniques that will be developed and used to carry out the research	The research activities will be mainly carried out on a modelling basis. The modelling of the CVI process will be based on the solution of transport equations of mass, momentum, species and energy in the gaseous phase using open-source frameworks (primarily OpenFOAM) and in-house libraries (such as OpenSMOKE++) in order to ensure the maximum level of flexibility and customization of solution algorithms. The densification process, i.e. the infiltration of pyrolytic gaseous products inside the preform pores and the subsequent deposition of graphitic carbon, will be modelled via transport equations of mass, momentum, species and energy in a porous

	material with properties evolving in time. Detailed kinetic mechanisms (including dozens of species and hundreds of reactions) will be considered in the resulting models, in order to ensure the highest level of accuracy of numerical simulations and reduce as much as possible the adoption of tuning parameters, derived from experimental observation. Proper numerical techniques will be conceived and implemented to manage the wide range of characteristic times characterizing the densification process, i.e. from ms (associated to the pyrolytic reactions) to days (which is the time required to complete 1 / 4 the densification). During the period spent abroad, the PhD candidate will have the opportunity to collect experimental data on lab-scale reactors, of significant relevance to validate and asses the quality of the numerical methodology. Brembo S.p.A. will provide experimentally measured data about specific CVI reactors currently adopted for production purposes (geometries, operating conditions, temperature field, densification curves, quality of deposited carbon, etc.), essential to test the developed computational methodology described above and to assess its limitations in cases of industrial interest. The developed tools will be adopted to explore the adoption of alternative reactor geometries, with the aim to improve the internal distribution of residence times (i.e. to avoid/reduce recirculation areas) and to reach more homogeneous conditions in terms of temperature and composition. More complex scenarios, based on unconventional operating conditions (for examples oscillation of reactor pressure) will be also investigated, with the objective to improve the quality of the deposited carbon. Thanks to the adoption of detailed kinetic mechanisms, the simulation results will be collected and analysed to extract knowledge about the impact of local operating conditions (temperature and composition) on the quality of the deposited carbon. Finally, during the internship period in Brembo S.p.A., a digital twin of a CVI reactor for industrial production will be developed, to help to mirror and monitor the production phase itself.
Educational objectives	The main educational objectives are: to reach a high level of knowledge and understanding of the CVI process and

	to master the skills and methods associated with it; ¿ to develop the ability for critical analysis, assessment, and synthesis of new and complex ideas; ¿ to extend the limits of what is currently known through innovative and high-quality work; to devise, design, and conduct research that has a real academic weight and a strong connection with the industrial world.
Job opportunities	The PhD candidate is expected to become a scientist/expert mastering the necessary tools and methodologies from a cross-approach perspective (theory, computation, and experimentation), making her/him the ideal profile for a position in Academia and Research Centers. At the same time, thanks to the exposure to the industrial environment and the strict connection with Brembo S.p.A., the PhD candidate will acquire critical and innovative spirit. teamwork ability, and project management skill, thus becoming especially attractive to companies investing in research and innovation, especially in the automotive, and energy sectors.
Composition of the research group	2 Full Professors 2 Associated Professors 2 Assistant Professors 6 PhD Students
Name of the research directors	Prof. Alberto Cuoci

Contacts
CRECK Modeling Labhttp://creckmodeling.chem.polimi.it/ alberto.cuoci@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	566.36 €
By number of months	6

National Operational Program for Research and Innovation

Company where the candidate will attend the stage (name and brief description)	Brembo S.p.A.
By number of months at the company	6
Institution or company where the candidate will spend the period abroad (name and brief description)	Nagoya University, Japan
By number of months abroad	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: - 2nd year: about 1.500 euros per student 3rd year: about 1.500 euros per student Teaching assistantship: availability of funding in recognition of supporting teaching activities by the PhD student: there are various forms of financial aid 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.