

3-years PhD position in CHANCE project

**IN-SITU and EX-SITU EXPERIMENTAL CHARACTERIZATION OF FLAME-MADE NANOPARTICLES AND NANOSTRUCTURED FILMS**

Description of the position

The PhD study is part of the CHANCE project (experimental CHARacterization of flame-made Nanoparticles and nanostructured films for Cfd dEvelopments), funded by OI PSINANO. The specific aim of the CHANCE project is to create the needed experimental and numerical framework for the fabrication of films with prescribed characteristics by in-situ deposition of pure and functionalized (doped) sensing materials via Flame spray pyrolysis (FSP).

Flame-Spray Pyrolysis (FSP) - at the core of this project - is based on the flash-evaporation of a solution - solvent plus precursors – sprayed as droplets into a flame to obtain nanoparticles. The process can be tuned to generate more complex particles, such as core-shell microstructure or nanocomposites. Among the different applications of nanoparticles, sensors or bacteria-resistant, self-cleaning, anti-fogging surfaces, just to mention a few, are characterized by the presence of a thick (several tens of micrometers) film composed by nanoparticles (commonly of ~ten nanometers). FSP technology represents an interesting alternative for large-scale production also of nanoparticle films with precise characteristics by suitably controlling the local conditions that particles will experience. Thus, disposing of simulations would be of great value, but requires validated CFD (computational fluid dynamics) models. For this, fundamental understanding of metal-oxide production and experimental database on academic flame configurations are still needed. Thus, the main objective of this thesis is to **experimentally characterize the production of TiO<sub>2</sub> nanoparticles and film deposit in laminar and turbulent H<sub>2</sub> flames by combining in-situ and ex-situ measurements.**

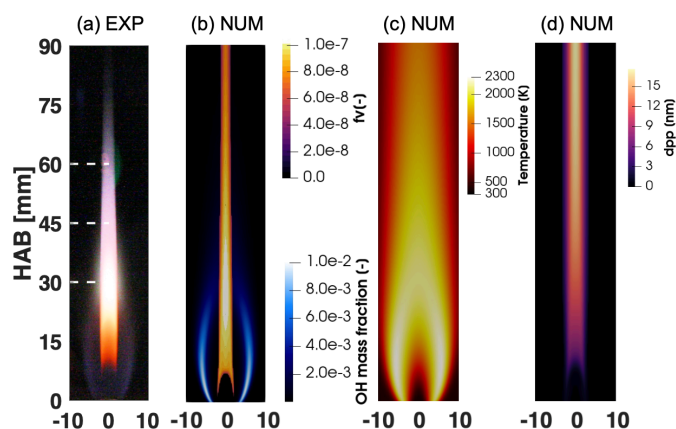


Figure 1 Comparison between the luminosity of an H<sub>2</sub>/air laminar flame producing TiO<sub>2</sub> nanoparticles (a) and (b-d) numerical results. For the simulation result (b), the volume fraction of TiO<sub>2</sub> is expressed with a yellow-red color bar, and the mass fraction of OH is expressed in blue color. Temperature (c) and mean primary particle diameter (d) are also provided [J. Yi et al. App. Energy Combust. Sci., 15:100190, 2023].

## Activities

We will focus on the production of TiO<sub>2</sub> nanoparticles to produce nanostructured films. For the configuration, a laminar H<sub>2</sub>/air flame where liquid nanoparticles (NP) precursors are pre-evaporated before injection will be considered. By doing so, turbulence and spray effects on NP production do not have to be considered. Specifically, the Yale diffusion burner (YDB) will be investigated experimentally. It consists of an inner tube for H<sub>2</sub>/N<sub>2</sub> gas injection with a diameter of 3.9 mm and a wall thickness of 0.5 mm and it is surrounded by a concentric air co-flow of a diameter of 50 mm. It allows the stabilization of a laminar co-flow diffusion flame. A thermalized version of the YDB burner with a pre-vaporized injection system has been developed at EM2C laboratory so that the liquid precursor (in this case TTIP, titanium isopropoxide) is fully evaporated in the fuel mixture before reaching the exit of the injection tube. The use of H<sub>2</sub> as fuel is motivated by the simplicity of its kinetics but also to explore its use for nanoparticle production as original application of future green hydrogen. This configuration will be the reference for the following steps:

- A) The laser-induced incandescence (LII) technique was recently applied to obtain the spatial evolution of the volume fraction of TiO<sub>2</sub> using an in-situ approach. In this thesis, new approaches will be developed to obtain additional information on the refractive index and the average size of primary particles from the spectral and temporal information of the LII signal.
- B) Characterization of size, morphology, crystal phase of nanoparticle population via ex-situ measurements at the height above the burner where the deposition substrate will be positioned in step C. Sampled TiO<sub>2</sub> nanoparticles will be counted using a scanning mobility particle sizer (SMPS) and analyzed with a transmission electron microscopy (TEM) to characterize their morphology and an X-ray diffraction (XRD) to determine the structure of the NP.
- C) Fabrication of nanostructured films and their characterization in terms of composition, structural form, and microstructure via scanning electron microscopy (SEM), XRD and TEM by considering different deposition times. For this, a system to position the substrate in a water-cooled block equipped with a thermocouple to control the substrate temperature will be developed.
- D) Finally, the potential of the developed approaches for TiO<sub>2</sub> production in turbulent flames will be explored.

## Skills

We aim to recruit a person that will characterise exhaustively the flame-synthesized powder and nanostructured films. Applicants for PhD appointment will hold a M.Sc. in Mechanical Engineering/Energetics. The position requires:

- Strong willing to develop experimental skills in the combustion field.
- Good oral and written communication skills to report, to present in congress and to write articles for scientific journals.

## Context

The successful candidate will have access to the most advanced experimental equipments for the investigation of solid particles production in flames from both EM2C and SMPS laboratories. On the one side, the burner envisaged for this work is already used at EM2C laboratory, together with the lasers, camera, SMPS and DMA facilities, classically used for the characterization of PSD of soot production in flames. The successful candidate will join the EM2C team working on the experimental and numerical characterization of (soot and metal-oxide) nanoparticles in flames, supervised by B. Franzelli, C. Betrancourt and J. Bonnetty. On the other side, the characterization of the nanoparticles and of the films will rely on the experience and equipment (DRX, TEM, SEM) of the team of G. Dezennau at SMPS laboratory.

## How to apply

For any information, please contact B. Franzelli at benedetta.franzelli\_at\_centralesupelec.fr.