JOB OFFER – THESIS

Modelling of Non-Equilibrium Plasma Discharges for Hydrogen Combustion

OFFER INFORMATION

Reference: E&S-24-NB-01
Team: E&S

Salary: 33 K€/year (gross)
Period: 3 years - from: 02/09/2024

Location: 42 Avenue Gaspard Coriolis – 31057 Toulouse
Contact person: Florent Duchaine & Nicolas Barléon

Required Level: Master

Key words : Computational Fluid Dynamics; Combustion; High Performance Computing; Hydrogen; Plasma

CERFACS

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HOSTING TEAM - E&S

The Energy & Safety team, formerly the CFD-Combustion team, focuses on cross-disciplinary activities aimed at developing, optimizing and deploying scientific codes dedicated to advanced combustion calculations in industrial geometries. The team focuses on the simulation of flows, applying them to aircraft, rockets, helicopters, car engines, turbines and more. The result is essential tools for a wide range of applications, with the leitmotiv: let's calculate systems before we build them. More specifically, team members develop models and tools covering chemical reduction, turbulence, combustion, two-phase systems, combustion instabilities, etc., to meet both academic and industrial challenges. Thanks to its position, the team collaborates with numerous scientific groups, design offices of Cerfacs associates, and other Cerfacs teams.

CONTEXT

A major challenge for our society is to ensure access to reliable energy with low impact on the climate and the environment. To this end, sustainably produced hydrogen (H2) is a carbon-free alternative to the fossil fuels used today. However, the use of H2 as a fuel requires the adaptation of current combustion chambers in order to maximise efficiency, limit the emission of nitrogen oxides (NOx), and ensure safety. NOx emission regulations require the use of lean or ultra-lean premixed combustion for H2, which raises ignition and flame stability issues. The objective of this Ph.D., as part of the JETHPAC project (funded by ANR french government), is to develop the use of plasma discharges, more specifically Nanosecond Repetitively Pulsed Discharges (NRPD), an excellent candidate to i) guarantee a timely ignition after H2 injection in the combustion chamber, and ii) control combustion instabilities.

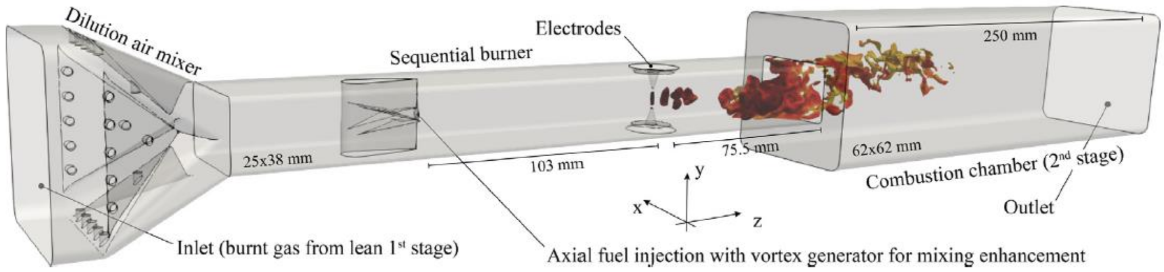
OBJECTIVES

The objective of this Ph.D is to understand how Non-Equilibrium Plasma (NEP) discharges can affects hydrogen combustion such as for ignition, flame stabilisation and pollutant emissions. For that purpose, the work has been divided in three major milestones, that have been defined to match with the measurements availability from the CAPS laboratory at ETH Zurich.

First, a thorough examination of the discharge in a flowing H2-air mixture will be conducted with both detailed chemistry tools (Cantera and Arcane)[1] and the AVBP code (http://www.cerfacs.fr/avbp7x) with its plasma extension[2, 3]. The chemical tools will be used to identify the major chemical pathways, based on idealised cases, that have to be retained in a reduced-order chemical model for Plasma-Assisted H2 Combustion (PAHC). One the other hand, detailed simulations of the plasma discharges in a cross flow will be used to investigate dimensional effects on the discharge properties. Then, the phenomenological model presented in [4] will be modified to account for the observations made from the simulations and experiments.

Second, Large-Eddy Simulation (LES) of Plasma-Assisted H2 Ignition in a flowing channel will be conducted using AVBP and the plasma LES closure developed in the first part of the Ph.D. Both flow parameters (velocity, turbulence, mixture, ...) and discharge parameters (frequency, energy, ...) will be investigated to provide recommendations for the use of NRP discharges for Plasma-Assisted H2 Ignition, both in term of reliability and safety.

Third, flame stabilisation will be investigated in a realistic burner shown in the figure below. Starting from a stable flame, acoustic forcing will be applied to study flame response to perturbations. NRPDs will be finally applied to investigate their potential to mitigate instabilities. Moreover, these simulations will be used to evaluate the impact of NRPD on NOx production that is a key issue in PAHC.



ORGANIZATION OF RESEARCH WORK (36 months)

The schedule of this Ph.D. is based on JETHPAC-ANR project with the following tasks:

<u>Task T1:</u> Literature Review Task: Simulation of Plasma-Assisted Combustion of Hydrogen
This task aims to conduct a comprehensive literature review on the simulation of plasma-assisted combustion of hydrogen. The purpose is to gather relevant research articles, conference papers, and scholarly publications to understand the current state-of-the-art, methodologies, findings, and potential areas for further research in this field.

<u>Task T2:</u> Plasma effects modelling
The objective is to improve the knowledge on the effects of NEP discharges of the NRP type on flowing H2-containing reactive mixtures. To do so, an important work will be carried out on the validation and analysis of a chemistry allowing to describe these conditions, revealing the relative part of the energy going to gas heating (fast and slow) and radical production. The validation will be performed by comparison with experiments from ETH Zürich. From a kinetic analysis, a phenomenological model will be developed and implemented into the AVBP Navier-Stokes solver within the Large Eddy Simulation (LES) framework as in Ref. [5].

In addition, detailed 3D plasma simulations of NRP discharges will be performed and compared with experiments. The specificities of discharges in a fast flow corresponding to a real burner will be studied. If they prove to be important for the physics of combustion, an adequate model will be developed.

<u>Task T3:</u> Plasma-assisted H2 ignition in a flowing mixture
The ignition mechanisms will be investigated numerically. Once validated by comparison with experiments, numerical simulation allows a precise analysis of the physics. Indeed, it gives access to the aero-thermochemical state of the reactive flowing mixture at any point in space and time. The phenomenological model developed in task T2 will be used to account for plasma impacts, resulting in thermal, kinetic and transport effects. As already performed in Ref. [6], some effects of the discharge such as the generation of radical species will be artificially inhibited to evaluate the impact of these effects on the ignition. Moreover, this numerical study will analyze the influence of flow perturbation levels on ignition probability.

<u>Task T4:</u> Mitigation of combustion instabilities
The ability of NRP discharges to stabilize combustors in regards to thermos-acoustics has been demonstrated using hydrocarbon fuels. The objective here is to assess the capacity for H2-air mixtures and to understand the physical mechanisms. For this, a straight channel including electrodes will be used. The flame will be anchored in the combustion chamber located downstream of this channel. In this configuration, acoustic perturbations will be artificially induced to mimic the loudspeakers used experimentally. The response of the H2 flame with and without NRPD will be quantified.

<u>Task T5:</u> Reduction of NOx emissions
A deep investigation of NOx formation will be performed all along the combustion chamber to understand the main production and destruction chemical pathways, based on the baseline simulations performed in Task T4 (non-acoustically pulsed flame with and without NRPD). A H2-air combustion chemistry mechanism including the chemistry for NOx using the ARCANE reduction tool will be derived. This mechanism must be able to retrieve NRPD effects on NOx, in addition to the conventional NOx routes evidenced in H2-air burners. These detailed 3D turbulent simulations will help to understand the complex formation mechanism of NOx in plasma actuated H2 flames.

<u>Task T6:</u> Writing
Capitalising on, promoting and mid-term reports and the thesis manuscript: the last task will involve a substantive activity carried out throughout the thesis aimed at capitalising on and synthesising the various works and advances. In particular, the doctoral student will have to provide annual intermediate reports and summary sheets, write publications and take part in conferences with an international audience and ensure the transfer of information and training to the Cerfacs. The writing of the thesis manuscript will be part of this task.

PLANIFICATION

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PROMOTING RESEARCH WORK

In order to obtain and enhance the value of the doctoral thesis, as well as to gain experience in the scientific community, the doctoral candidate must publish their work in internationally renowned scientific journals. Additionally, the doctoral candidate must also participate in international conferences (such as PROCI, GEC) and possibly one or two national or European conferences. The objective is to gain recognition for the doctoral research and contribute to the visibility of the hosting laboratories (CERFACS) within the international scientific community.

TRAINING

Several training sessions at Cerfacs have been identified for the first year of the thesis on the essential numerical tools required for the thesis work: AVBP, Cantera, Arcane, Antares, Centaur, and LES simulation.

DESIRED PROFILE

- Master's degree (or equivalent) in a relevant academic field (Mechanical, Energy or Chemical Engineering or closely related).
- Must have great interest and be willing to work in the field of multi-physics combustion, with a focus on zero-carbon fuels, gas-turbine technologies, and related disciplines, including physics.

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HOW TO APPLY ?

To apply, please send your CV and covering letter to duchaine@cerfacs.fr or barleon@cerfacs.fr, applications are open until 31/08/2024.

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REFERENCES

[1] L. Cheng, N. Barleon, B. Cuenot, O. Vermorel, A. Bourdon, Plasma assisted combustion of methane-air mixtures: Validation and reduction, Combustion and Flame 240 (2022) 111990.
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[6] M. Castela, B. Fiorina, A. Coussement, O. Gicquel, N. Darabiha, C. O. Laux, Modelling the impact of non-equilibrium discharges on reactive mixtures for simulations of plasma-assisted ignition in turbulent flows, Combust. Flame 166 (2016).