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THESIS PROPOSAL - Fixed-term contract
Investigation of chemical pathways in hydrogen combustion

Reference: CFD-2023-CUE-03
Team: CFD
Research unit: Energetics and propulsion
Salary: 33.6 K€/year (gross)
Duration: 36 months - **Starting date**: From February to September 2024
Level of education required: Master of science

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HOST LABORATORY

The **Cerfacs** is a fundamental and applied research center specializing in modelling and digital simulation. Through its resources and expertise in high-performance computing, it addresses major scientific and technical problems in public and industrial research. The Cerfacs teams develop innovative methods and software solutions to meet the needs of the aeronautics, space, climate, energy and environment sectors. Cerfacs works in close interaction with its seven associates: **Airbus**, **Cnes**, **EDF**, **Météo France**, **Onera**, **Safran** and **TotalEnergies**.

JOB DESCRIPTION

Topic(s): Molecular Dynamics Kinetics Combustion Hydrogen Plasma

Context:

The rising importance of hydrogen combustion in the context of decarbonization, particularly within the aerospace and energy production sectors, is evident. The potential challenges related to combustion instability are expected to emerge as a primary concern with these new hydrogen engines, like what has been experienced in the past with kerosene engines, particularly when aiming for lean combustion regimes to reduce NOx emissions. To address these challenges, disruptive solutions have to be found accompanied with the development of numerical tools linking fundamentals to applied physics.

Mission:

This project aims at investigating the chemical pathways of hydrogen combustion in a range of conditions relevant to practical applications. The study will be based on molecular dynamics simulations and will attempt to assess and quantify the chemical pathways leading to:

- the formation of NOx
- catalysis at walls in hydrogen-air combustion system.

The study will be performed in collaboration with Imperial College and Penn State University. The current molecular dynamics framework will be used to build reaction kinetics to be included in CFD simulations of lab-scale experiments. Developments of reactive molecular dynamics may be necessary to improve the accuracy and robustness of the simulations. The specific objectives of the project are to:

- understand and assess the NOx emissions of hydrogen systems
- understand and assess possible catalytic effects at walls of hydrogen systems
- provide accurate reaction kinetics of the formation of NOx and wall catalysis in hydrogen combustion and, depending on the progress of the project, hydrogen-plasma assisted combustion

Expected Results:

- New knowledge on the chemistry paths, energy barriers of nitrogen oxide formation and wall catalysis in hydrogen-air systems
- New reaction kinetics of nitrogen oxide formation and wall catalysis in hydrogen-air systems
- Evaluation of NOx and catalysis effects in lab-scale experiments with hydrogen combustion and hydrogen-plasma assisted combustion.

The PhD position is part of the ICHAruS project (DC2 - https://icharus.eu/), a MSCA doctoral network funded by the European Community. The project brings together leading research institutions in Europe, industrial partners and international universities to develop innovative technologies for the safe and efficient utilization of hydrogen in transportation and power generation. The Ph.D. candidate will participate to network-wide training activities, workshop and conferences, along with secondments periods in network partners' laboratories.

Application must be done following the procedure detailed at: https://euraxess.ec.europa.eu/jobs/177738.

DESIRED PROFILE

Background required:

Numerical simulation | Chemical Physics | Programming Python/Fortran/C++

Abilities:

Capacity for analysis and synthesis **Innovation capacity** **Ability to work independently**
Relational qualities **Rigorous**