

JOB OFFER – STAGE

High-fidelity numerical simulations of thermo-chemically inhibited flames

OFFER INFORMATION

Reference: E&S-25-OD-02 Location: 42 Avenue Gaspard Coriolis – 31057 Toulouse

Team: E&S

Supervisors:

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Gratification: 800€ net per month - M2 level or last year at engineering school

Period: 6 months - from: 02/03/2026

Key words: flame inhibition, two-phase flow simulations, flame/particle interaction

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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

To tackle the global energy crisis, hydrogen appears as a potential solution to replace fossil fuels. On a national level, the hydrogen sector is particularly well supported, with a strong ambition for 2030 to develop green, totally carbon-free hydrogen (52% by 2030, compared with 5% in 2020, for various sectors: industry, mobility, energy) [Fra-25]. Nevertheless, these initiatives are facing complex safety challenges inherent to hydrogen, during production, conversion, transport, and use. Due to the broad flammability limits, low minimum ignition energy, and high chemical reactivity, hydrogen fire and explosion accidents can occur frequently. For instance, from 2000 to 2020, more than 90 incidents in the hydrogen industry were recorded [Che-22]. The growing use of hydrogen between now and 2030 will automatically increase these risks. Prevention measures do exist and aim at limiting the risk of ignition or explosion (typically, leak detection combined with venting and recombination for open and



confined enclosures, respectively). However, these solutions have proven to fail in certain cases, leading to ignition with catastrophic consequences. This realization leads to the conclusion that novel mitigation techniques are urgently needed.

Deflagration inhibition is a promising technique, which relies on the injection of substances capable of reducing the chemical reactivity of flammable mixtures and reduce the flame acceleration phase responsible for the severity of the explosion scenario. Despite its scientific interest and practical importance, inhibition of H₂-containing deflagrations is essentially uncharted territory, because of the lack of fundamental knowledge about the mechanisms governing the complex interaction between inhibiting particles (liquid or solid) and fast-propagating deflagrations. An illustration of the large-scale interaction of accelerating flames with inhibiting particles is provided in Fig. 1.

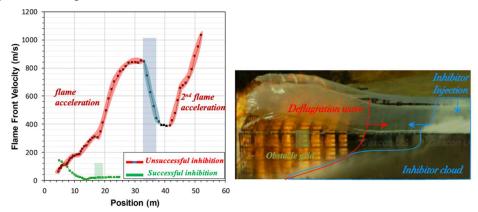


Figure 1: (right) Illustration of the large-scale interaction of an accelerating flame with inhibiting particles. (left) evolution of the flame speed with flame position in two different tests. Green curve shows a successful inhibition (drastic reduction in flame speed), red curve is a test case where particles are able to induce a local inhibition effect (blue region) but are not able to prevent flame acceleration. The mechanisms controlling the efficiency of the inhibition technique are still unknown today and are at the center of the ANR project **CHAIN-H2**.

The ANR project **CHAIN-H2** is a collaboration between CERFACS, ICARE and ASNR, and aims at using advanced experimental and numerical techniques to extend the current knowledge on these mechanisms. This internship position is focused on the numerical part and will develop advanced numerical techniques to investigate the processes governing flame/inhibiting particles interaction.

A Phd position is also associated to this internship, provided the candidate demonstrates strong research skills and a genuine interest in the subject.

MISSION

In light of this context, the internship objective is to extend the capabilities of *a particle-resolved DNS code* to accurately reproduce the complex interaction of flame fronts with a set of inhibiting particles. The problem is illustrated in Fig. 2 and will consist on a planar flame interacting with water droplets.

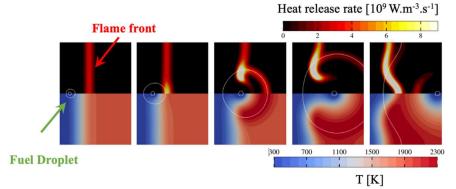


Figure 2 : Illustration of the transient Fuel droplet/flame interaction. This internship will replace fuel droplet by water droplet and investigate its mitigating effect on the flame front.



The internship will focus on H2/air flames mitigated by water droplets as a simple example of inhibiting particles acting on flames via a purely thermal mechanism (evaporation and convective heat transfer). The internship will also focus on H2/air flames. The following scientific program is envisaged:

Scientific program:

- The two-phase flow solver is already available but lacks the necessary thermo-chemical coupling between the flow and the particles. The first task of this internship will therefore be focused on coupling the two-phase flow solver with a thermo-chemical solver called CANTERA. CANTERA will be used here to update the flame/particle thermo-dynamic properties as well as the chemical source terms needed for flame chemistry.
- 2. These developments will be validated against a simple test case of a H2/air flame interacting with an isolated water droplet as illustrated in Fig. 2 (with the fuel droplet replaced by water droplet). The capacity of the water droplet to locally mitigate the flame front will be studied.
- 3. The impact of key flame and droplet parameters on this mitigating effect will also be investigated.

DESIRED PROFILE

- Master's degree (M2) or engineering school
- Background in fluid mechanics and energy
- Training in CFD (Computational Fluid Dynamics)
- Knowledge of combustion and/or plasma is a plus
- Programming skills (Fortran, C, or C++ and Python)

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HOW TO APPLY?

To apply, please send your CV and covering letter to <u>dounia@cerfacs.fr</u> and <u>guodong.gai@toulouse-inp.fr</u>, applications are open until 15/12/2025.

See you soon at CERFACS!