Scuola Superiore Meridionale

MERC PhD Project Proposal 2024/2025

H_2 Spontaneous Ignition: Fundamentals and Risk Mitigation

Project description

Hydrogen, due to its high reactivity, low ignition energy, and wide flammability range, poses unique challenges in fire and explosion safety. In particular, jet fire scenarios—involving high-velocity, high-pressure hydrogen leaks igniting into flames—require thorough understanding and accurate modelling to ensure safe design and risk mitigation in hydrogen production, storage, and transport systems.

One of the main issue in H_2 jet fire scenario is the uncontrolled ignition. In all conditions of high pressure hydrogen release, it has bene observed and immediate ignition
without any apparent ignition source present like spark, hot surfaces, fires…[1, 2].

Starting from the pioneering work of Wolanski and Wojcicki in 1972, many studies both experimental and model/theoretical have been developed.

Astbury and Hawksworth (2005) reviewed the possible mechanisms identified for spontaneous ignition: temperature increase due to the reverse Joule-Thomson effect, the electrostatic charge generation, the impact of shock induction during the diffusion of leaked hydrogen., the ignition by shock waves, the sudden adiabatic compression... [3]

Experimental works provide critical conditions of the phenomenon, however the test results are quite dependent on the experimental conditions and the experimental setup and then they are not able to give insights into the mechanisms driving the phenomenon.

Recently, advanced models have been developed to study the role of the mechanisms affecting the spontaneous H_2 ignition [4, 5].

In addition, the influence of the main operating (pressure, temperature, composition) and design (tube length and diameter, obstacles…) conditions has been investigated.

In all the models present in the literature, the interaction between the jet and the shock waves has been simulated and identified as the mani mechanism affecting spontaneous ignition.

The role of radicals generation and detailed kinetic mechanism has been never investigated in details.

The aim of this project proposal, is to underly the physical and chemical phenomena affecting the spontaneous ignition of high pressure jet of hydrogen, by taking into account the coupling of fluid dynamic and detailed kinetic mechanism.

To this end, advanced mathematical models of different complexity for simulating the spontaneous ignition of high pressure jet of hydrogen, will be developed.

The key question of this project is: **are we sure that the phenomena identified in the literature driving the hydrogen spontaneous ignition are able to explain the phenomena? Is there a role of the reaction mechanism?**

OBJECTIVES

Objective 1 - Develop a model and simulate spontaneous ignition of hydrogen-air by including only the effect of detailed reaction mechanism, at varying pressure, temperature, composition.
Objective 2 - Simulate ignition and flame propagation using CFD tools coupled with detailed hydrogen-air reaction mechanisms.
Objective 3 - Identify critical parameters influencing the ignition delay and flame stabilization (e.g., jet velocity, temperature, equivalence ratio, pressure…).
Objective 4 - Compare simulation results with experimental data from literature or laboratory tests to validate the models.

METHODOLOGIES

To achieve the above objectives, the research project is organized in Tasks.

Task1 – Rank and literature review of all the mechanisms
A detailed review of the results, both experimental and model, on spontaneous ignition will be performed. Based on the literature results, The role of each mechanism will be analyzed in details.

Task2 – Reaction mechanism based model
The simulations of spontaneous ignition of H_2/air mixtures by only modelling the role of detailed reaction mechanism will be performed at varying temperature, pressure and equivalence ratio.

Task3 – Advanced CFD model and validation
Based on the results of the previous task, an advanced CFD model will be developed to fully characterize the interaction between the fluid flow, the detailed kinetic mechanism and the shock wave propagation. CFD models of different complexity will be developed, also in collaboration with prof. Poinsot form CERFACS research center. The model results will be validated against the literature experimental results.

Task4 – Model validation
Conclusion on risk mitigation strategies will be derived from the obtained results.

Relevance to the MERC PhD Program

The proposed project deals with Risk in Industrial Processes and also to Complexity, as it will be performed by the development of advanced models (CFD coupled with detailed reaction mechanism).

The disciplines relevant to this project are the following:

1) *Risk analysis – engineering, analysis and management of risks*
The aim of the project is understating the mechanisms for optimising risk mitigation of high pressure accidental H_2 release.

2) -Mathematical modelling and simulation of complex systems

To perform detailed simulations of spontaneous ignition a complex mathematical model has to be developed which takes into account the coupling between turbulent fluid flow generated by the high pressure hydrogen jet and the detailed kinetic mechanism. The model should simulate the complex phenomena resulting from the interaction between turbulence and combustion, posing significant issues in terms of mathematical modelling and numerical solution.

Commitment on mathematical modelling and chemical/physical models of turbulent combustion flows and numerical issues will be demanding.

Key references

[1] Li H, Cao X, Liu Y, Shao Y, Nan Z, Teng L, Peng W, Bian J. Safety of hydrogen storage and transportation: an overview on mechanisms, techniques, and challenges. Energ. Rep. 2022;8:6258–69. https://doi.org/10.1016/jegyr.2022.04.067

[2] Jiang Y, Pan X, Cai Q, Klymenko OV, Wang Z, Hua M, Wang Q, Jiang J. Physics of flame evolution following spontaneously combusting hydrogen emerging from a tube into the unconfined space. Combust. Flame. 2023;251:112683. https://doi. org/10.1016/j.combustflame.2023.112683.

[3]Astbury G.R., & Hawksworth S.J. Spontaneous ignition of hydrogen leaks: A review of postulated mechanisms. 2005. Proceedings of The 1st International Conference on Hydrogen Safety

[4] Xin-Yi Liu , Z.Y. Sun, Yao Yi , Progress in spontaneous ignition of hydrogen during high-pressure leakage with the considerations of pipeline storage and delivery, Applications in Energy and Combustion Science, Volume 20, December 2024, 100290).

Joint supervision arrangements

Supervisor is:
Prof. Almerinda Di Benedetto – University of Naples Federico II will support the whole PhD activity.
Every 2 weeks the PhD student will meet with supervisor.

Location and length of the study period abroad (min 12 months)

Supervisor: prof. Thierry Poinsot, Research Director

Institute : Institut de Mécanique des Fluides de Toulouse, CNRS
Université de Toulouse
1 Allee du Professeur Camille SOULA
Toulouse 31400 Cedex , France

Agreement is in preparation.

Any other useful information

-