

Application for the 20th ERCOFTAC da Vinci Competition

Title of PhD thesis: Modeling Strategy for the Large Eddy Simulation of Lean Hydrogen-Air Explosions

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Summary for General Public

Hydrogen is expected to play a major role in the energy transition, but its widespread adoption raises serious safety challenges. In particular, hydrogen-air mixtures can be highly flammable and lead to violent explosions in confined or semi-confined environments, making accurate predictive tools essential for risk assessment. My PhD focused on the **prediction of hydrogen-air explosions** using **Large Eddy Simulation (LES)** — a computational approach that captures the interaction of turbulent flows with combustion. I developed a new modeling framework that improves the reliability of LES for hydrogen safety applications. The work spans **fundamental flame physics**, captured through high-fidelity simulations of small-scale flame instabilities, up to **realistic-scale explosion scenarios** such as the **ENACCEF2 facility**, representative of industrial risks. The goal is to provide better tools for designing and securing hydrogen-based energy systems.

Scientific Summary

Motivation and Industrial Context (LEFEX Project)

This work was carried out within the **LEFEX project**, an industrial partnership between CERFACS, TotalEnergies, Air Liquide and Natran (formerly GRTGaz). The project aims to improve hydrogen safety modeling for future energy infrastructures (e.g. refueling stations, storage and transport facilities). Accurately predicting the **pressure loads** and **flame propagation** in case of accidental ignition is a central industrial concern.

However, classical Large-Eddy Simulation (LES) models often fail when applied to **lean hydrogen-air mixtures** because of their **sub-unity Lewis number** and strong **sensitivity to flame stretch** and **thermo-diffusive instabilities**. These effects, though crucial for flame acceleration and overpressure prediction, are either filtered or amplified in conventional modeling strategies such as the **Thickened Flame (TF)** model.

Methodology - From DNS to LES: A Multi-Scale Approach

Understanding the flame dynamics underlying hydrogen-air explosions requires investigating their most fundamental behaviors. To this end, I began with **Direct Numerical Simulations (DNS)** of **spherical lean hydrogen-air flames**, which resolve all relevant physical and chemical scales. These simulations revealed the early development of **thermo-diffusive instabilities**, leading to the formation of **cellular flame fronts** characteristic of sub-unity Lewis number mixtures (cf. *Figure 1*).

While DNS provides invaluable physical insight, it is prohibitively expensive for real-world geometries. To simulate **practical explosion scenarios**, I turned to **Large Eddy Simulation (LES)** — a computational approach that resolves large-scale turbulent structures while modeling small-scale effects. In reactive flows, LES commonly uses the **Thickened Flame (TF)** model, which artificially increases flame thickness to make it numerically tractable.

However, for **hydrogen flames**, especially at lean conditions, the TF model can become inaccurate. These flames are (1) highly sensitive to stretch and (2) intrinsically unstable under the thermo-diffusive mechanism due to their sub-unity **Lewis number ($Le < 1$)**. I identified and addressed two key issues in the TF approach:

1. The **amplification of flame stretch effects**, which arises due to the artificial thickening of sub-unity Lewis number flames;
2. The **filtering of thermo-diffusive instabilities**, which suppresses essential flame front dynamics at typical LES resolutions (cf. *Figure 1*);

Both mechanisms result in a strong dependency to mesh resolution for the TF model, thereby questioning its predictive capabilities (cf. *Figure 2*).

To overcome this, I proposed a **generalized modeling framework** designed to improve the predictability of LES for lean hydrogen-air explosions. The proposed strategy, called **Thermo-Diffusive-Stretched-Thickened Flame (TD-S-TF)** model, introduces two **complementary corrections**:

1. A treatment to **mitigate the stretch amplification** artificially introduced by the TF model;
2. A subgrid model to **represent the overall effect of unresolved flame front instabilities**.

These corrections were first developed and validated on **canonical configurations** (cf. Figure 2), methodically extended and later applied to **realistic explosion scenarios** (cf. Figures 3-4), demonstrating improved accuracy and reliability in reproducing flame dynamics and overpressure development.

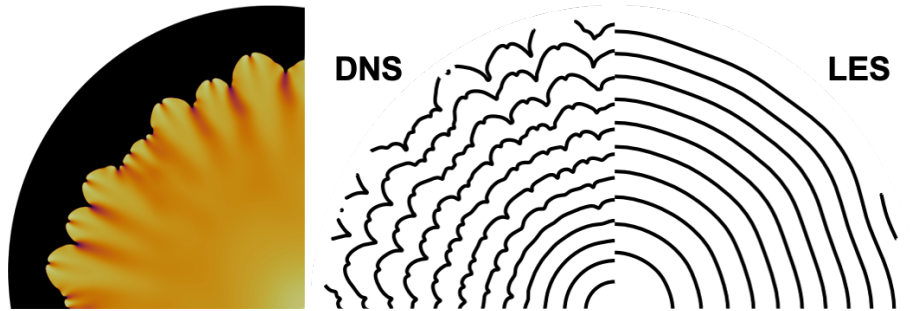


Figure 1. Comparison of lean H₂-air spherical flame propagation: **DNS (left: temperature field, middle: isotherms at several instants)** reveals thermo-diffusive instability structures; **LES (right: isotherms at several instants)** with standard TF fails to capture them.

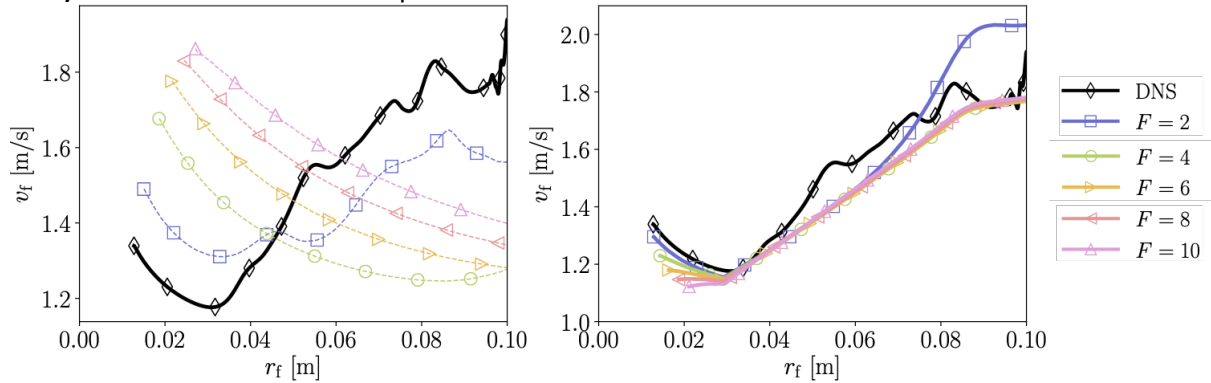


Figure 2. Flame speed as a function of flame position in the spherical set-up: **standard TF model (left)** vs. **TD-S-TF model (right)**. Reference DNS is in black. TD-S-TF curves correctly reproduce DNS propagation, while TF exhibits a strong mesh dependency.

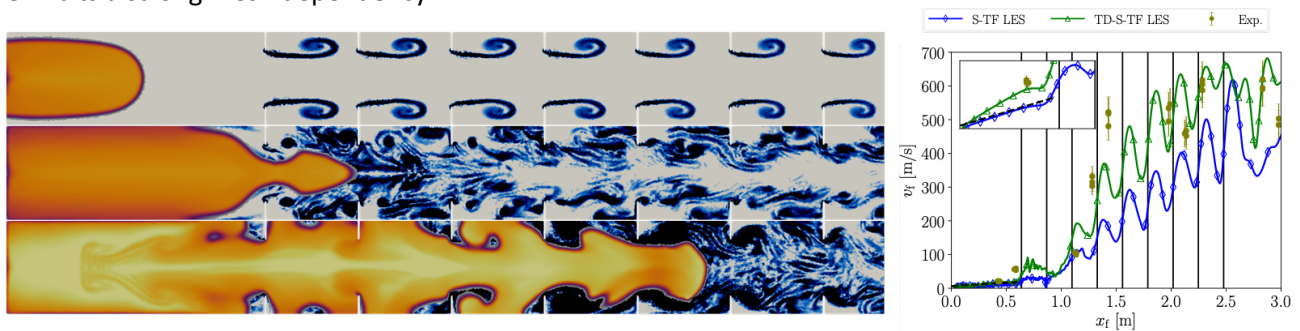


Figure 3. Left: snapshots from LES of the ENACCEF2 explosion using the **TD-S-TF model** at 3 different stages, showing temperature (red-orange colormap) and vorticity (blue colormap) fields. Right: flame tip velocity vs. position in ENACCEF2: comparison between S-TF (stretch correction only), TD-S-TF (full correction) and experimental data (symbols with error bars). TD-S-TF curve correctly captures the experimentally measured propagation.

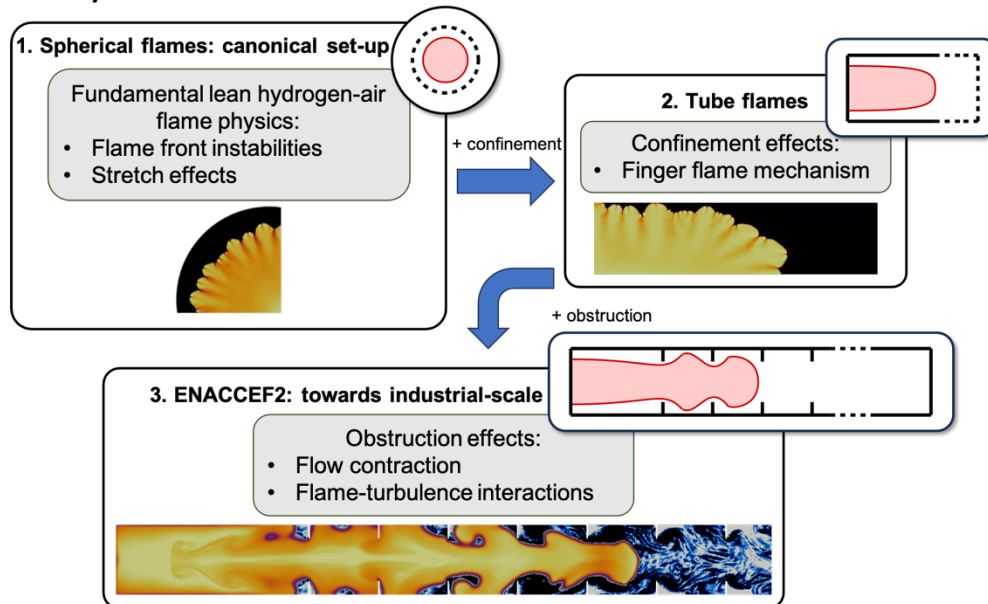
Novelty and Applicability in Engineering

The key novelty lies in the **integration of fundamental combustion physics (flame stretch, instability, Lewis number effects)** into an engineering-compatible LES framework. While such effects are well-known in academic combustion studies, they are rarely included in practical simulations due to modeling complexity.

My TDSTF model bridges this gap, allowing engineers to simulate hydrogen explosions **more accurately** without excessive computational cost. This is crucial for hydrogen infrastructure design, where safety margins are tight and accurate risk assessment is mandatory.

Moreover, the model has been tested for a wide range of operating conditions, on set-ups of increasing complexity, ranging from canonical flames to industrial-scale applications, spanning 1D, 2D and 3D set-ups. It is **modular and extensible**, making it adaptable to other fuels or combustion regimes, including ammonia or blended hydrogen mixtures. It represents a step forward toward **predictive LES** in safety-critical applications.

Graphical summary



Selected Publications

1. Hok, J.-J., Dounia, O., Vermorel, O., & Jaravel, T. (2022). *Effect of Flame Front Thermo-Diffusive Instability on Flame Acceleration in a Tube*. Proceedings of the 28th International Colloquium on the Dynamics of Explosions and Reactive Systems, 1–6.
2. Detomaso, N., Hok, J.-J., Dounia, O., Laera, D., & Poinso, T. (2023). *A generalization of the Thickened Flame model for stretched flames*. *Combustion and Flame*, 258(December), 113080.
3. Hok, J.-J., Dounia, O., Detomaso, N., Jaravel, T., Douasbin, Q., & Vermorel, O. (2024). *A modeling strategy for the Thickened Flame simulation of propagating lean hydrogen-air flames*. *International Journal of Hydrogen Energy*, 78(July), 1133–1141.
4. Hok, J.-J., Dounia, O., & Vermorel, O. (2025). *A thickened flame model extension for the simulation of lean hydrogen-air explosions in confined environments*. *Combustion and Flame*, 275(February), 114070.
5. Matas Mur, E., Hok, J.-J., Dounia, O., & Douasbin, Q. (2025). *A posteriori Evaluation of the Stretched-Thickened Flame Model for Accurate LES of Hydrogen Flames*. Proceedings of the 12th European Combustion Meeting, 1–9.

Total Output Volume

- 6 peer-reviewed publications
- 5 conference presentations
- 345-page thesis manuscript
- 2 ongoing collaborations with industrial partners
- Implementation in industrial LES solver