Towards the large-scale modeling of turbulent combustion in fast deflagrations

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1 Introduction

In industrial safety, the prevention of gas explosions and the mitigation of their effects is a major concern. This is not only the case for the process industries, but also for the energy and transportation sectors. These hazards are at the origin of human casualties and injures, material losses, as well as business disruption, all with potentially catastrophic consequences. Industrial explosions killed more than 500 people between 2010 and 2015 [?]. In the same period, in the hydrocarbon industry alone, the associated cumulated property damage losses associated with incidental events were of over 5 billion US dollars [?]. These hazards may even lead to social and political ramifications that may far exceed direct financial damages. This is the case for hydrogen for example whose rising importance in the industry in the last years is facing serious safety concerns that may jeopardize its role in the energy transition. This is due to several explosion incidents all around the word in the recent years: in 2019 alone, three hydrogen explosion incidents occurred within 20 days around the world: a refuelling station, a transport vehicle and a storage tank explosion [1]. These incidents and more recent ones [2], emphasize the need for accurate and reliable tools to assess the risk of hydrogen explosions.

The increase in computational ressources in the last decades has allowed to perform predictive 3D numerical simulations of gas explosions in increasingly larger-scale environments, thanks to the Large-Eddy-Simulation (LES) method [3–14], making these 3D-LES an essential tool for the design of mitigation strategies to reduce the severity of these hazardous events. These 3D-LES have also allowed an in depth analysis of the flame acceleration mechanisms that lead to the emergence of fast deflagrations, a regime often associated to severe explosion events. Their predictive capabilities, however, depend largely on the accuracy of their constitutive turbulent combustion models, which have been shown to need serious revisiting when used for hydrogen containing mixtures [15], especially in very lean conditions. In these conditions, hydrogen flames are prone to small scale flame front instabilities and we show in this paper that accounting for their impact on flame acceleration and their intricate interaction with turbulence is of paramount importance for the accurate prediction of the processes leading to fast deflagrations.

2 Fast deflagration test case

The configuration studied here is the ENACCEF-2 acceleration tube detailed in [20, 21] and illustrated in Fig. 1. It is a closed, cylindrical, vertically oriented tube with identical and evenly spaced annular

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obstacles. It is 7.65 m-long, with an inner diameter of 230 mm. The spacing between obstacles is equal to 230 mm. All the obstacles have the same inner diameter of 140mm and a thickness of 4 mm, yielding a blockage ratio of 63%. The first annular obstacle is placed 640 mm away from the ignition plate and the last one at 2480 mm. The remaining tube is obstacle-free. Several operating conditions have been studied in this setup [20, 21], comprising variable compositions and initial temperatures (homogeneous and with gradients). Here, three atmospheric and homogeneous lean hydrogen/air mixtures are studied, containing 11%, 13% and 15% of H2 in volume. This corresponds to equivalence ratios of $\phi = \{0.29, 0.36, 0.42\}$ respectively.

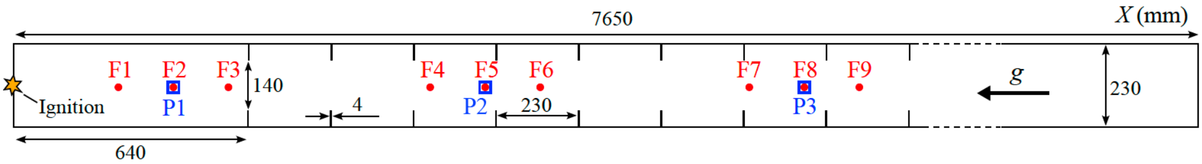


Figure 1: Schematic of the cross section of the cylindrical ENACCEF-2 setup [20, 21]. Dimensions are indicated in millimetres. The axial positions of the photomultipliers (F) and the pressure transducers (P) are provided. The tube is vertically installed and the flame is ignited at the bottom of the tube.

The mixture is ignited at the center of the bottom end of the channel. The obstruction in the tube provides a very strong, jet-type, flame acceleration that yields fast deflagrations at the end of the tube, reaching flame propagation speeds in the range $[400, 600]\, m/s$ for these mixtures [20, 21], which are about $10^3 - 10^4$ times their associated fundamental consumption speed s_L^0. This strong flame acceleration and the very lean hydrogen/air mixtures considered (prone to flame front instabilities) make ENACCEF-2 a particularly challenging test case for the turbulence combustion models used in LES, as will be highlighted in the next sections.

3 Numerical setup

The LES are performed using the massively parallel solver AVBP [22] developed at CERFACS. The second order in space and time, Lax-Wendroff advection scheme [23] is used. The LAD selective filter is applied on the pressure field [24] to detect discontinuities corresponding to shocks and to apply second order artificial diffusion. Gravity effects are also included in the LES, although its effect is negligible in the ENACCEF2 setup. Regarding the mesh, a uniform resolution of $\Delta x = 4\, mm$ is imposed until the exit of the obstructed section of the tube ($X < 3\, m$) where FA takes place, and a coarser resolution of $\Delta x = 10\, mm$ is used downstream. It is important to note that focus is put here on the obstructed region only. Flame propagation in the obstacle-free region is not discussed in this paper. Additionally, the mesh is refined around the lip of the annular obstacles, to obtain a resolution of five points in their width, yielding $\Delta x = 0.8\, mm$. This ensures a proper resolution in the region responsible for the generation of the vortical and turbulent structures involved in FA. Further mesh sensitivity tests have been performed in [19], validating the present mesh configuration. In this paper, the WALE model [25] is used for the subgrid-scale turbulence.

3.1 Boundary conditions and initialization

The channel being entirely closed, all boundary conditions are walls. An isothermal boundary condition is employed, with the temperature being set at the ambient initial value $T_{wall} = 296\, K$. A law-of-the-wall approach is retained since the mesh resolution employed is not sufficient to resolve the turbulent boundary layers induced by the high velocity flow during the explosion. The simulation is initialized with a quiescent, homogeneous hydrogen/air mixture of the corresponding composition, in the whole domain. The explosion is initiated through a hemispherical kernel of burnt gases. The center of the kernel corresponds to the position of the spark ignition in the experiments. Close to the ignition kernel, a velocity profile is established, so that mass conservation though the flame and zero-velocity boundary condition at the walls are verified.

3.2 Chemistry modeling

A global single-step formalism fo the chemistry is retained: $2H_2 + O_2 \to 2H_2O$, with an associated chemical source term $\dot{\omega} = C_{O_2}^{n_R/2} C_{H_2}^{n_R/2} Aexp(-Ea/RT)$. Regarding species transport, a constant Lewis number approach is used. For each mixture, a set of parameters for the chemical source term and transport properties are obtained using the 1S-LeFit procedure described in [16, 17, 19] to match the flame speed, thickness and response to stretch of a complex chemical scheme of reference (UCSD). They are provided in Table 1.

Table 1: Singe-step chemical source term and species transport parameters used in this paper.

ϕ	s_L^0 (m/s)	δ_L^0 (μm)	T_b (K)	$n_R/2$	Ea (kcal/mol)	A (cm^3/mol/s)	Le_{O_2}	Le_{H_2}	Le_{H_2O}
0.42	0.290	515	1469	0.563	36.719	2.514×10^{11}	1.662	0.4709	1.217
0.36	0.134	850	1322	0.315	46.987	8.735×10^{9}	1.517	0.4300	1.112
0.29	0.0289	2800	1167	0.315	46.987	4.825×10^{9}	0.9749	0.2763	0.7143

3.3 Stretch sensitive flames and the (S-TF) model

The first part of the combustion modeling deals with the insufficient resolution in LES-type meshes to solve for the flame internal structure. This is done by using the thickened flame approach [26], (TF) in Eq. (1). By multipliying thermal and species diffusivities (D_{th} and D_k resp.) and dividing the species chemical source terms $\dot{\omega}_k$ by a factor $\boldsymbol{F}$, it allows to thicken the flame front by this same factor $\boldsymbol{F}$ while preserving the fundamental laminar flame speed s_L. Inside the flame front, $\boldsymbol{F}$ is given by ($\boldsymbol{F}\delta_L = N_c \Delta x$), where δ_L and Δx are the flame thickness and mesh size respectively, which allows to resolve the flame on N_c grid points ($N_c = 7$ in this paper). $\boldsymbol{F} = 1$ in regions outside the flame front.

$$\text{(TF):}\; \begin{array}{l} D_{\text{th}} \mapsto \boldsymbol{F} D_{\text{th}} \\ D_k \mapsto \boldsymbol{F} D_k \\ \dot{\omega}_k \mapsto \boldsymbol{F}^{-1} \dot{\omega}_k \end{array} \;;\; \text{(S-TF):}\; \begin{array}{l} D_{\text{th}} \mapsto \boldsymbol{F} D_{\text{th}}, \\ D_k \mapsto \boldsymbol{F}_{\text{sp}} D_k, \\ \dot{\omega}_k \mapsto \boldsymbol{F}_r^{-1} \dot{\omega}_k, \end{array} \tag{1}$$

The problem with the thickening procedure is that it amplifies the effects of stretch on the consumption speed in stretch-sensitive flames, including hydrogen flames [17, 18]. A solution to this problem is provided in [17, 18], (S-TF) in Eq. (1), and consists in a Lewis changing procedure ($\boldsymbol{F}_{sp} \neq \boldsymbol{F}$) that allows to match both the fundamental flame speed (using $\boldsymbol{F}_r$) as well as the flame response to stretch (controlled by $\boldsymbol{F}_{sp}/\boldsymbol{F}$). It is shown in [17,18] that (S-TF) efficiently solves the strong mesh-dependancy observed with the TF approach when used against very lean hydrogen flames including those studied in this paper.

3.4 Two approaches for the subgrid-scale modeling of very lean hydrogen combustion in deflagrations

The most challenging aspect in the LES of deflagrations lies in the necessity to accurately account for: (1) the laminar processes controlling the early stages of flame acceleration; (2) the turbulent combustion regime reached a certain distance from ignition; and (3) the transition between the first and second regimes. Very lean Hydrogen deflagrations are particularly challenging in that regard since: (i) it is shown in [17, 18] that their propensity for flame front instabilities strongly enhances flame acceleration and must therefore be accurately taken into account; (ii) their associated thermo-diffusive effects have an intricate interplay with turbulence, which must be accounted for in turbulent combustion models as highlighted in [15]. To showcase the importance of the accurate modeling of (i) and (ii), two approaches for the subgrid-scale modeling of very lean hydrogen combustion will be confronted to the experimental results of ENACCEF-2.

Independence Hypothesis Approach (IHA) In this approach, flame front instabilities are modeled using the correlation $\boldsymbol{E}_{\text{TDS}}$ of Goulier [28] which was validated in combination of the (S-TF) model against early stage flame acceleration cases (spherical propagation [17] and finger flame acceleration [18]). This is expected to yield good results during the first, laminar phase of the explosion ($X < 640mm$), which precisely corresponds to a smooth tube propagation (finger flame). Turbulent combustion is modeled using the efficiency function $\mathcal{E}$ from Charlette et al. [27]. The (IHA) approach Eq. (2) assumes that TD effects are decoupled from turbulence and that they are well represented by flame front instabilities observed in laminar, spherically expanding flames, regardless of the combustion regime of the flame. The turbulent speed simply reads $s_T = \mathcal{E}\boldsymbol{E}_{\text{TDS}} s_L$. Note that the S-TF approach is retained and is here used to correct the amplification of stretch effects by the thickening procedure.

$$\text{(IHA):} \quad \begin{array}{r} D_{\text{th}} \mapsto \mathcal{E}\boldsymbol{E}_{\text{TDS}}\boldsymbol{F}D_{\text{th}}, \\ D_k \mapsto \mathcal{E}\boldsymbol{E}_{\text{TDS}}\boldsymbol{F}_{\text{sp}}D_k, \\ \dot{\omega}_k \mapsto \mathcal{E}\boldsymbol{E}_{\text{TDS}}\boldsymbol{F}_r^{-1}\dot{\omega}_k, \end{array} \Longrightarrow \begin{array}{l} \delta_L \mapsto \boldsymbol{F}\delta_L, \\ s_T \mapsto \mathcal{E}\boldsymbol{E}_{\text{TDS}}s_L \end{array} \tag{2}$$

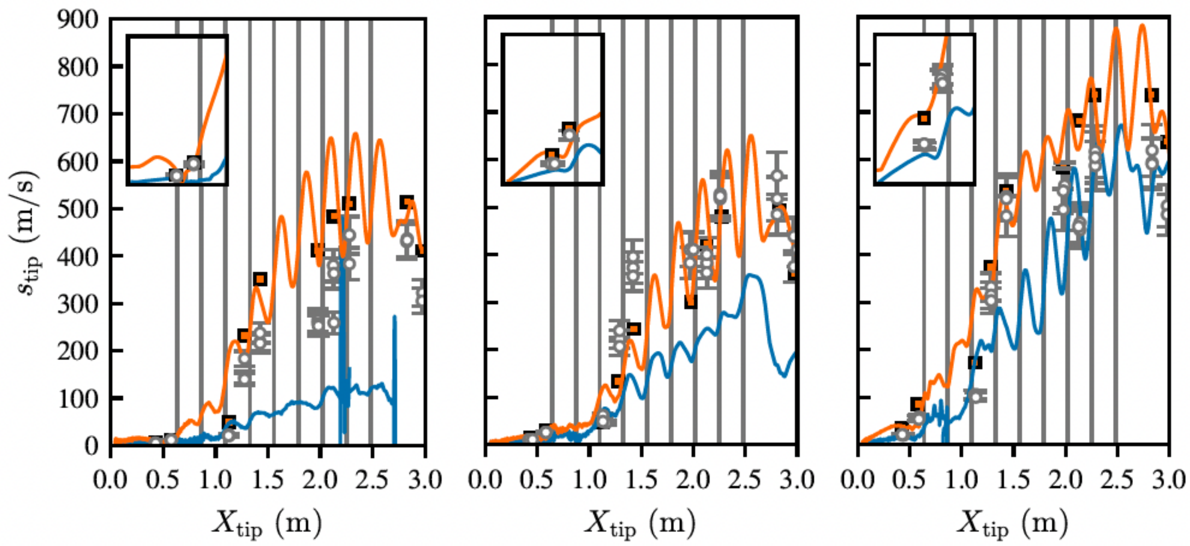
The accuracy of such pragmatic approach for the prediction of very lean hydrogen deflagrations is worth assessing for its straightforward implementation in CFD codes. It has also been used in engine combustion chambers applications [29].

Fractal modeling of very Lean Hydrogen Turbulent Combustion (FLHTC) The second approach gets rid of the independence hypothesis which was shown to not hold for all turbulent levels in recent DNS of very lean and turbulent hydrogen flames [15]. In it, a model was proposed based on the decomposition of the turbulent speed as $s_T = \Xi_\Delta I_0 s_L^0$, where Ξ_Δ is a fractal model for the flame surface wrinkling in turbulent very lean hydrogen flames proposed in [15] and I_0 is a stretch factor which accounts for the thermo-diffusive effects inducing variation of the local flame consumption in stretched flames, for which a correlation proposed in [30]. The S-TF approach is also used here to correct the amplification of stretch effects by the thickening procedure.

$$\text{(IHA):} \quad \begin{array}{r} D_{\text{th}} \mapsto \Xi_\Delta I_0\boldsymbol{F}D_{\text{th}}, \\ D_k \mapsto \Xi_\Delta I_0\boldsymbol{F}_{\text{sp}}D_k, \\ \dot{\omega}_k \mapsto \Xi_\Delta I_0\boldsymbol{F}_r^{-1}\dot{\omega}_k, \end{array} \Longrightarrow \begin{array}{l} \delta_L \mapsto \boldsymbol{F}_{\text{th}}\delta_L, \\ s_T \mapsto \Xi_\Delta I_0 s_L \end{array} \tag{3}$$

4 Interplay between thermo-diffusive effects and turbulence in the very lean deflagrations .

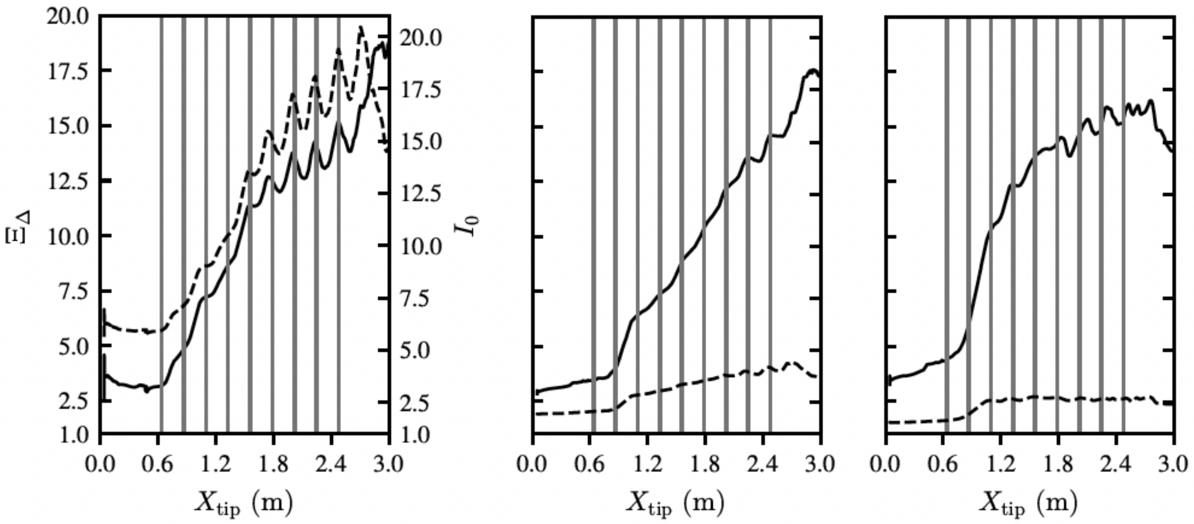
The two approaches to subgrid-scale modeling of very lean hydrogen combustion are confronted against the flame speed experimental data of ENACCEF-2 in Fig. 2. While the (IHA) strategy allows to reasonably predict the flame speed at the final stage of flame acceleration for the richest mixture, its inability to accurately predict flame acceleration is increasingly striking as the mixtures become leaner. On the other hand, the (FLHTC) modeling strategy clearly outperforms the (IHA) approach for all cases considered, highlighting the importance of taking into account the positive interaction between turbulence and thermo-diffusive effects to reproduce flame acceleration in very lean hydrogen deflagrations. (FLHTC) is shown here to be the most appropriate modeling choice regardless of the mixture composition.



(a) $\phi = 0.29$ (b) $\phi = 0.36$ (c) $\phi = 0.42$

Figure 2: Absolute flame tip speed s_{tip} with respect to the flame tip position (in the X axis) for the three mixtures considered. The LES (solid lines) are compared to three experimental realizations (symbols). The results obtained with (IHA) are shown in blue while those obtained with (FLHTC) are shown in orange. Discrete values of flame speed for the LES, obtained through a similar procedure as the experiments, are indicated by squared symbols. The obstacles are indicated by vertical lines. An inset figure shows a zoom in the first 870 mm of the tube, up to $s_{tip} = 80m/s$.

The evolution, along the flame propagation, of the contribution of both Ξ_Δ and I_0 are displayed in Fig. 3 for all three ENACCEF2 mixtures. Before the first obstacle, both Ξ_Δ and I_0 remain roughly constant, accounting for laminar TD effects. Then, they increase along the obstructed section of the tube, as a result of flame/turbulence interactions. However, while the quantitative values of subgrid-scale flame surface wrinkling Ξ_Δ are similar in the three mixtures, the values of subgrid scale stretch factor I_0 strongly vary with the composition. The values of I_0 and their increase along the flame propagation are larger for leaner mixtures. Values as high as $I_0 \approx 20$ are reached in case $\phi = 0.29$, indicating an increase of four times with respect to initial, laminar values. These results are coherent with the drastic increase in stretch sensitivity of hydrogen flames as leaner conditions are reached.



(a) $\phi = 0.29$ (b) $\phi = 0.36$ (c) $\phi = 0.42$

Figure 3: Evolution with flame propagation of averaged values of Ξ_Δ (left axis, solid line) and I_0 (right axis, dashed line) along the flame brush.

5 Examples of Figures and Tables

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