Effect of Flame Front Thermo-Diffusive Instability on Flame Acceleration in a Tube

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1 Introduction

Being decarbonated, hydrogen stands as an interesting candidate to reduce greenhouse gas emissions. However, its storage and transport in big quantities raise safety concerns. Following a leakage, mixed with the surrounding air, this hydrogen can form a highly flammable mixture. In case of accidental ignition of the hydrogen/air premix, different combustion scenarios and regimes are possible, depending on factors such as geometry (dimensions, presence of obstacles), mixture composition, temperature, pressure or turbulence level. These regimes range from slow deflagration to the transition to detonation in the worst case. However, even in the absence of a transition to detonation, the overpressure generated by the acceleration of the flame may threaten the integrity of people and facilities.

One specific case of interest for safety studies is the explosion scenario in a tube. This environment is indeed particularly conducive to flame acceleration leading to significant damage. The mechanism of flame propagation in tubes is well-documented. Among all, the studies of Bychkov et al. [1] and Valiev et al. [2] show three important properties of the early stages of flame propagation in tubes : (1) a flame acceleration phase is observed in the first instants after ignition; (2) this acceleration stage is limited in time and ends when the flame reaches the side walls; (3) the acceleration rate is inversely proportional to the tube radius.

The present study focuses on premixed mixtures of air and small concentrations of hydrogen, representative of leaks for instance. In these lean conditions, thermo-diffusive flame front instabilities are expected to develop. Indeed, the Lewis number of lean hydrogen-air mixtures is less than unity. It means that the unbalance between thermal diffusion of heat and molecular diffusion of reactants will lead to a flame instability enhancing the combustion processes and the flame acceleration. Following the pioneering work of Bechtold and Matalon [3] and Frankel and Sivashinsky [4], which gave the fundamental equations of linear stability theory, other papers provide more theoretical [5, 6], experimental [7, 8] and numerical [9, 10] investigations of flame front instabilities. These studies have all been conducted in canonical configurations such as planar flames and outwardly propagating spherical flames.

However, subunity-Lewis number flames in tubes will undergo the competing effects of both aforementioned acceleration mechanisms. Grosseuvres [11] and Katzy [12] have shown qualitatively from experimental measurements that flame front thermo-diffusive instabilities play a major role in the early propagation phase of a flame ignited in a tube. The question is now: how are both phenomena coupled ?

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The objective of the current paper is to provide a numerical study of the interplay between these two flame acceleration mechanisms: thermo-diffusive instabilities and finger-flame effects.

2 Numerical methods

It is usually agreed upon that thermo-diffusive instabilities result in cellular structures at scales ranging down to the flame thickness [9]. Due to computational cost constraints, Direct Numerical Simulations (DNS) of 3D tubes are impractical. Therefore, a 2D configuration is retained. A schematic of a characteristic set-up is depicted in Figure 1. A symmetry is imposed at the bottom to reduce the computational domain to half-a-tube. A slipping (resp. non-slipping) adiabatic condition is set on the left (resp. top) wall while an outlet is imposed at the right end to mimic the rest of the tube. The left side velocity assumption is meant to avoid any initial flame wrinkling at the wall which would force the development of thermo-diffusive instabilities. Instead, a free-slip hypothesis ensures they can appear anywhere along the flame surface. The length of the tube is chosen twice as long as the diameter to allow for finger-flame development without influence of the outflow condition. The flame is artificially ignited by imposing a hot kernel of burnt gases on the bottom left corner of the domain. Its radius is set to 1 mm for all cases, lower than the critical radius for the onset of instabilities which is estimated around 9 mm [13]. This value also ensures that the initial flame kernel can be considered perfectly spherical, devoid of the lateral walls confinement effect.

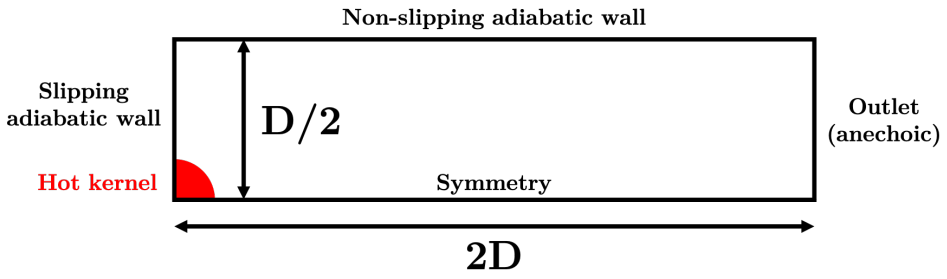

Figure 1: Schematic of tubes dimensions.

The chosen operating point corresponds to the exprimental conditions used by Grosseuvres [11] for which flame front instabilities are observed: homogeneous hydrogen-air mixture at $\Phi = 0.356$, $T_u = 296$ K, $P = 1$ atm.

To study the relative importance of thermo-diffusive instabilities versus finger-flame acceleration effects, three geometries are considered by varying the tube radius R_{tube} (while keeping the same aspect ratio). Each geometry is characterized by its adimensional radius defined as the ratio of R_{tube} over the flame diffusive thickness $Pe_{tube} = R_{tube}/l_f$. A summary of the different configurations is presented on Table 1.

Table 1: Test cases.

Name	Tube radius $\mathbf{R_{tube}}$ (mm)	Tube length (mm)	$\mathbf{Pe_{tube}}$
Tube S	54.2	216.8	250
Tube M	108.4	433.7	500
Tube L	216.8	867.4	1000

As for the chemistry, a 1-step scheme (four species, one reaction) following an Arrhenius law has been chosen. The advantage of such a scheme is to allow a direct choice of the Lewis number for species

involved in the global reaction whilst avoiding the complexity of intermediate species. To understand the interaction between flame instabilities and finger-flame effects, two chemistries are constructed. The first one assumes $Le_k = 1$ for each species k (noted "Le1") and allows a quantification of pure finger-flame propagation without any instability. The other uses realistic Lewis number values (noted 'LeRe'), retrieved from simulations using the detailed San Diego chemical scheme [14]. In both cases, the pre-exponential constant of the Arrhenius expression is tuned in order to fit the laminar flame speed to the San Diego chemical scheme [14]. The computations of laminar flame characteristics are performed using the CANTERA open-source code, yielding: $s_L^0 \approx 12$ cm/s (laminar flame speed), $T_{ad} \approx 1320$ K (adiabatic flame temperature), $\delta_{th} \approx 850$ µm (flame thermal thickness) and $l_f \approx 217$ µm (flame diffusive thickness).

To perform the DNS, quadrilateral meshes for the 3 tube diameters are generated with a resolution of about 85 µm, allowing around 10 grid points in the flame thermal thickness to resolve the instabilities. The 2D tube simulations are performed using AVBP [15], an in-house code developed at CERFACS solving the multi-species compressible Navier-Stokes equations on unstructured grids using parallelization for high-performance computing (HPC).

3 Results and discussion

3.1 Lewis number effects in the tube S configuration

The role of thermo-diffusive instabilities can be first highlighted by comparing the instantaneous flow fields over time for the two chemistries and for a given pipe diameter. Figure 2 depicts isotherms at $T = 600$ K computed every 10 ms using either the unitary Lewis (top) or the realistic Lewis scheme (bottom) in the tube S set-up. While the former front remains smooth throughout the propagation, the latter wrinkles soon after ignition. Significant flame acceleration results from this wrinkling as it substantially increases the flame surface area and thus the total reaction rate. This is evidenced by the increasing spacing of isocontours in the LeRe case.

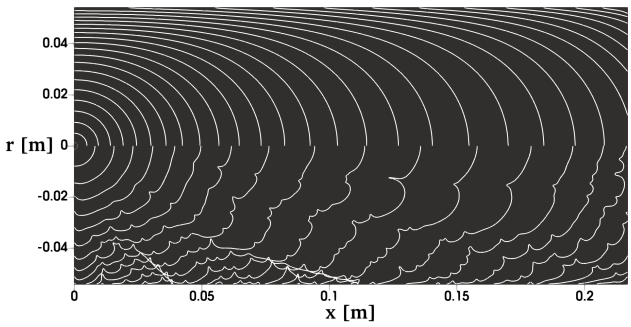

Figure 2: Snapshots of $T = 600$K-isotherms every 10 ms in the tube S. Le1 scheme (top) and LeRe scheme (bottom).

To assess more quantitatively the effect of instabilities on the propagation, the flame front speed v_{tip} is extracted, with the flame front position x_{tip} defined as the most advanced point in the tube in the x direction on the isotherm $T = 600$ K. Figure 3 shows the flame propagation in the $v_{tip} - x_{tip}$ frame. The kinematic model of Bychkov et al. [1] is represented by the dashed black line. According to their analysis:

$$v_{tip} = \sigma s_L^0 + \frac{s_L^0}{R_{tube}}(\sigma - 1)x_{tip} \tag{1}$$

where $\sigma = \rho_u/\rho_b$ is the thermal expansion parameter (ρ_u and ρ_b are respectively the unburnt and burnt gases density). The simulation with unitary Lewis chemistry follows properly that trend. This confirms that Bychkov's theory is valid for unitary Lewis mixtures. Furthermore, the flame decelerates around $x_{tip} = 0.16$ m, when the flame "skirt" touches the lateral walls. At that moment, the flame surface shrinks, explaining the strong speed reduction. On the other hand, during the first phase when the flame is far from lateral walls, the LeRe case exhibits a larger acceleration rate. It means that the flame front instabilities have a significant effect on the propagation. While the front still has an almost constant acceleration rate, as expected in the theory, the value of this acceleration is about twice as big compared to the Le1 case. It should also be noted that in this figure, the two curves do not start from the same initial flame speed. Indeed, the LeRe case starts at a greater velocity, due to stretch effects in the early spherical propagation. However, this phenomenon is rapidly overtaken by thermo-diffusive and finger-flame effects which contribute more significantly to flame acceleration.

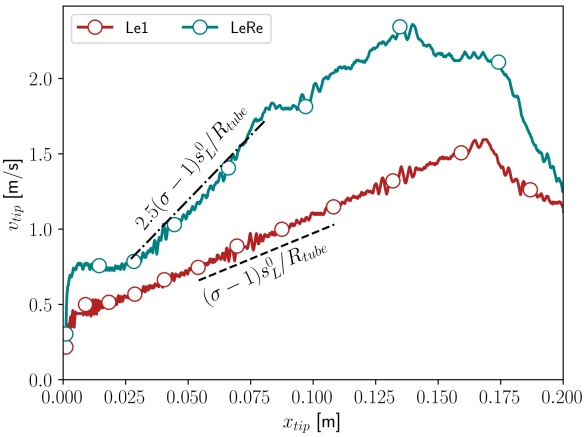

Figure 3: Flame front kinematic speed against flame front position in the tube S configuration. Dashed black line: asymptotic finger-flame acceleration slope [1]. Dot-dashed black line: 2.5 times the asymptotic finger-flame acceleration slope.

3.2 Competition between instabilities and finger-flame effects

To evaluate the prevalence of the effects of instabilities over finger-flame theory, flame kinematics for different tube radii are compared. Flame speeds are non-dimensionalized by s_L^0 to get s_{tip} whereas positions are divided by the tube radius R_{tube} to define ξ_{tip}.

First, the analysis in this non-dimensional $s_{tip} - \xi_{tip}$ phase-space on Figure 4 clearly demonstrates the similarity of all Le1 cases which collapse on a single curve. Indeed, following Equation 1, the asymptotic acceleration rate of the flame front in this space depends only on the thermal expansion ratio σ, namely:

$$s_{tip} = \sigma + (\sigma - 1)\xi_{tip} \tag{2}$$

To quantify the additional flame acceleration due to the thermo-diffusive instabilities described in Section 3.1, Figure 5 represents the flame tip non-dimensional speeds for the LeRe simulations divided by those obtained for the corresponding Le1 cases. Black stars on each curve denote the moment the flame skirt reaches the wall. It comes out that the influence of the instabilities depends on the tube radius. The larger the tube, the stronger the contribution of the instabilities to the flame acceleration. Indeed, widening the tube gives more room for instabilities to develop whereas the confinement effect of lateral walls weakens.

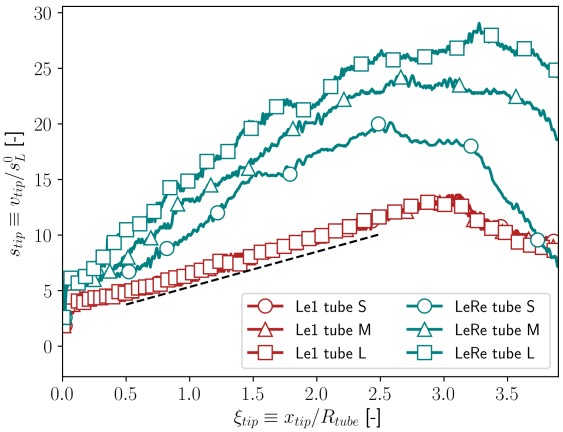

Figure 4: Non-dimensional flame front speed against non-dimensional position for several tube radii. Dashed black line: finger-flame acceleration slope [1].

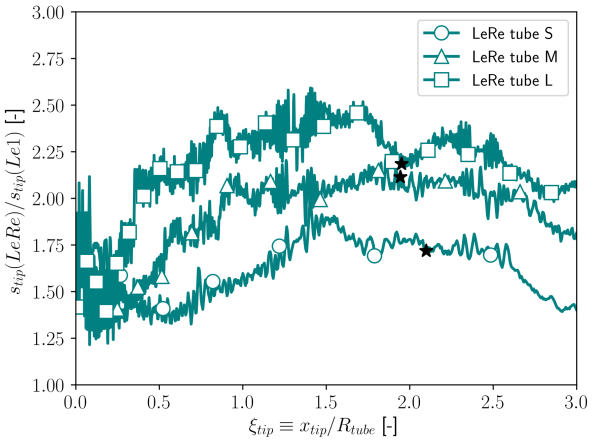

Figure 5: Non-dimensional flame speed for the LeRe cases divided by the corresponding Le1 cases against non-dimensional position for several tube radii.

4 Conclusion

Lean H_2-air flame propagation in a tube has been studied in order to understand the effect of flame front instabilities on flame acceleration occurring for mixtures at $Le < 1$. The comparison of simulations using unitary versus realistic Lewis numbers has given evidence for the additional acceleration due to the instabilities. Indeed, while the unitary-Lewis flames stay smooth and follow the finger-flame theory, the realistic-Lewis cases quickly form cells that contribute to combustion enhancement by supplementary wrinkling. A quantitative analysis has demonstrated that for a given tube radius, the acceleration rate of the thermo-diffusively unstable flame is considerably larger than that of the stable one. Besides, a variation in the tube radius has allowed for an analysis of the competing effects of instabilities and finger-flame. While small tubes are sufficiently narrow for finger-flame influence to be stronger than that of instabilities, larger tubes leave a broad channel in which instabilities develop longer before the flame takes on a tubular shape. It has also been shown on a similarity analysis that flame acceleration induced by the instabilities depend not only on the flame position, but also most importantly on the tube size. This means that, while conventional models developed in the spherical flame framework may be applicable to the initial short spherical phase, they cannot easily be extended to the finger-flame stage without a proper inclusion of the tube radius influence. Finally, it is worth mentioning that the current study of finger-flame and thermo-diffusive competition has been carried out by varying the tube radius, thus affecting the former effect. A perspective for future works would be to keep a single geometry and vary the chemistry so as to modify the thermo-diffusive influence.

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