DNS Study of Stabilization of Turbulent Triple Flames by Hot Gases

C. Jiménez¹ and B. Cuenot²

- (1) CIEMAT, Avda. Complutense, 20, 28040 Madrid, Spain.
- (2) CERFACS, 42 Av. G. Coriolis, 31057 Toulouse, France.

Abstract

Direct numerical simulations of turbulent flames stabilized by hot gases are presented and analysed with the aim of investigating the mechanisms which control turbulent flame stabilization. Even if the simulations are run on an idealized 2D configuration and use a simplified formulation, with single-step chemistry and Le=1 assumptions, they are useful in giving insight in the dynamics of flame stabilization. The current flames are stabilized by instantaneous reignition events triggered by hot gas convected by recirculation, which ignites lean premixed pockets that eventually produce a new triple flame upstream of the otherwise downstream travelling unsteady flame. While the occurrence of these events depends on the level of turbulence imposed to the flame, away from these occasional events the instantaneous flame propagates at a speed given by laminar flame properties, independent of the level of turbulence. This could explain why in some experiments [14] no correlation is found between the local turbulent intensity and the flame propagation speed, but a correlation is found between the mean flame position and the turbulence intensity.

Keywords: DNS, turbulent triple flame, flame stabilization

1. Introduction

Recent spectacular advances in computer technology and numerical techniques have made Direct Numerical Simulations (DNS) a widely used tool in combustion research and the user community more and more demanding in what concerns the complexity of these calculations. State-of-the-art simulations are three dimensional, use high order accuracy and include as much physics as possible, in particular detailed transport and thermodynamics, detailed chemistry,... (see for example [1]). However, rather

simple DNS of flames can still be very useful in understanding the dynamics of combustion and developing combustion models, and is used here.

The study focus in the dynamics of diffusion flame stabilization in turbulent flows. While flames stabilized by recirculation of hot combustion products are investigated, some of the results should be of general applicability to otherly stabilized flames, where the same mechanisms are present.

Earlier theories of lifted flame stabilization regarded these flames as either fully premixed or non-premixed. It was first proposed [2] that the

propagation speed of premixed flames governed the stabilization, which would occur in a point where the mean flame speed matched the flow velocity. In a second theory [3] the flame was assumed to stabilize in the stoichiometric surface point in which the dissipation (or strain) rate was below the quenching value. It seems now widely accepted that in the core of the stabilization mechanism stand the structures known as tribrachial or triple flames, which are established when some degree of partial premixing allows the formation of a lean and a rich premixed branch which burn partly the reactants, and a diffusion flame where the excess reactants are finally burnt downstream. Much theoretical [4-6], experimental [7, 8] and numerical [9–12] work has been devoted to the study of these flames. Even if results of measurements agree with this picture of flame stabilization, direct detection of instantaneous triple flames is difficult and insufficient to understand the mechanisms which control propagation speed and stabilization height in turbulent flames.

Recent work by Su et al. [13] proposed a mechanism for flame stabilization in a turbulent jet in which large scale structures play a major role: in their experiment they find that combustion does not affect the velocity or scalar fields upstream of the flame, but that the flame places itself preferentially in low incoming velocity regions. The flame has there enough relative speed to propagate upstream, and towards the fuel rich central-jet zones, where it encounters higher inflow velocities which make it propagate downstream until a richer large scale structure makes it again go towards leaner, lower velocity locations. These results are in some contradiction to the model proposed by Upatnieks et al. [14], which find no correlation between the flame speed and the passage of large scale structures, or between flame speed and local turbulence. They propose instead a picture in which, as suggested in [9], the combustion process modifies the velocity field, generating low velocity regions into which the flame can always propagate, provided that strain is not too strong. In this picture the flame would not see the incoming turbulence, and would remain almost laminar.

Experimental measurements have certain difficulties in assessing these theories. For example, it is difficult to identify the effects of large structures, as simultaneous measurements of the flame position and the passage of large structures are needed. This is a context where DNS, even in simpler formulations, can be of great help.

2. Description of the simulations

The flow configuration chosen to study stabilization is a mixing layer of diluted methane (CH4 20%, N2 80% in volume) and air in which a laminar diffusion flame is stabilized after a sudden expansion by a hot gas pocket (see Fig. 1). To simplify the calculation, the hot gas pocket is simulated here by an additional layer of hot inert gas, meant to replicate the energy supply effect of recirculating hot combustion products. Asymptotic analysis [15] describes the stabilization process by which a triple flame is installed, and is used here to construct initial conditions for the simulation. Because of the presence of hot gases in the air side, ignition of the lean branch is enhanced, and the triple flame has a characteristic " λ " shape (see Fig. 1).

The simulations are run by solving the fully compressible conservation equations for mass, momentum, energy and chemical species in a two dimensional cartesian domain with 200x300 grid points, using high order compact differences and a third order explicit Runge Kutta method, with a code described in [16]. Transport properties are simulated via a Sutherland law for viscosity and Schmidt and Prandtl numbers = 0.75 (thus equal diffusivities for the species and Le=1). A one step global mechanism for methane combustion was used here, with reaction rate given by $\dot{w}_F = A[Y_F][Y_O]exp(-E_{act}/RT)$, with $A=4.410^{23}$ (cgs units) and $E_{act}=50$ kcal/mole.

A well-known drawback of one step mechanisms when used for the study of triple flames is the overestimation of flame speeds for rich mixtures, which results in the rich branches being too long and propagating too fast. As a result of the geometry of the present configuration, the stoichiometric point and the lean premixed branch play the main role in the stabilization of the flame. A comparison of planar flame speeds at different stoichiometries obtained with the present one step mechanism and with GRI3.0 shows that, even if simple and detailed chemistry speeds differ, on the lean side ($\phi < 1$) the global mechanism is good enough for our purposes (see Fig. 2).

Once the laminar flame is established, a turbulent velocity field is injected through the inlet at a constant inlet mean velocity U (equal for the fuel and air inlets), using an unsteady, multi dimensional version of the NSCBC boundary conditions in which the transversal terms are taken into account when computing the characteristic wave amplitudes [17]. This 2D isotropic turbulent velocity field is generated by random fluctuations with a Passot-Pouquet spectrum and with the smallest scales of the order of 3 times the grid size, or about 0.14 time the air inlet size. Three different flame simulations, with varying injected turbulence intensity were run: in FLAME I, the turbulence level, given by the rms of velocity fluctuations measured with the mean velocity is u'/U = 0.1, in FLAME II

u'/U = 0.2, and in FLAME III u'/U = 0.4. Turbulence modifies the flame shape by several means: it enhances mixing, leading to ignition at locations closer to the inlet, but it also introduces strain in the flame, which can eventually lead to local extinctions. To avoid the propagation of the turbulent flame upstream and its attachment to the inlet boundary, the mean inflow velocity U is chosen to be $3.5S_L$, slightly higher than the maximum flame propagation speed detected in turbulent triple flames, which is about $3S_L$ [7, 8]. In the present configuration, a recirculation zone is created in the hot gas layer, which produces detachment of hot gas pockets, convected upstream and towards the air layer. Because of the presence of this hot gas reservoir, no extinctions are detected in the present simulations, not even at the highest turbulence levels. The effect of turbulence is in the three cases to enhance mixing and earlier ignition, with the instantaneous flames located closer to the inlet than the laminar flame. Occasional reiginition events are detected on the leaner side, when a hot gas pocket approaches a flammable mixture, which then propagates towards the stoichiometric mixture and lead to the formation of multiple triple point flames, as in the sequence presented in Fig. 3. In this sequence a hot pocket ignites the mixture upstream of the flame (a), this premixed combustion pocket propagates then downstream and towards richer zones(b), and when it crosses the stoichiometric line it produces a new triple point (c), then a third one (d), which finally merges with the original triple flame (e), resulting in a single triple flame (f).

3. Dynamics of the triple flames

DNS allows access to simultaneous instantaneous values of the different intervening variables. One can then attempt the description of the dynamical behavior of the instantaneous flames, and identify the stabilization mechanism. Dynamics of the stabilization is governed by the dynamics of the triple or edge point, defined as the point where the premixed branches and the diffusion flame meet, therefore a procedure for unambigous identification of this point is needed.

The triple point has been usually identified with the maximum heat release point in the flame. This is certainly the case if only one triple point exists at a given time. But it is evident from the plots in Fig. 3 that this criterium is not useful in the case of the present turbulent flames, as several triple points can be simultaneously present. Fernandez-Tarrazo et al. [12] used recently a different criterium in which the triple point was identified as the crossing point of the stoichiometric line and a line of constant temperature, which they chose

to be 1200K (a value intermediate between the fresh gases temperature T_0 and the adiabatic flame temperature T_{ad}). In Fig. 3 long–dashed white lines have been traced marking the stoichiometric contour and short–dashed white lines mark the isotemperature line corresponding to $T_i = T_0 + .5(T_{ad} - T_0)$. The crossing points of these lines coincide with the triple points even at those times in which several of them are found in the flame.

Once a method for detection of the triple points has been selected, their propagation velocity can be easily measured. First, the flame velocity with respect to the laboratory-fixed reference system can be computed as the time variation of the position of the triple(s) point(s):

$$\vec{u_f} = d\vec{x}/dt. \tag{1}$$

Then, the propagation speed with respect to the local flow can be computed as the difference between $\vec{u_f}$ and the gas velocity measured at the triple point $\vec{u_q}$:

$$\vec{u_p} = -(\vec{u_f} - \vec{u_g}), \tag{2}$$

with a minus sign so that it is positive when the flame propagates towards the inlet and the fuel side.

Also, the propagation speed along the stoichiometric line and in the direction normal to it can be easily obtained as:

$$u_{p_t} = \vec{u_p} \cdot \vec{t}, u_{p_n} = \vec{u_p} \cdot \vec{n}, \tag{3}$$

where \vec{n} and \vec{t} are the normal and tangential vectors to the stoichiometric line at the triple point.

Figure 4 presents a plot of the position in the x and y axis of the first (most upstream) and last (most downstream) triple points along the simulation for flames I, II and III. Most of the time, a single triple point is detected and both lines coincide. Only occasionally, after reignition events as the one described above, several triple flames coexist, and the first and last triple point are clearly separated. After an initial advance, all the flames appear to recede towards the outlet (higher x), except when reignition events create a new flame tip upstream. Displacement in the v axis appears to be uncorrelated to the advance/recession in the x axis. As a matter of fact, the position in y is driven by the turbulent flow, as can be seen in Fig. 5, in which it is shown to be correlated to the gas velocity in y direction, (only flame II is shown but the correlation appears in all the flames), while position in x is only slightly correlated to the gas velocity, if at all.

Both the mean x position (represented by dotted lines in Fig. 4), and its range of variation

depend on the imposed global turbulence intensity, with positions varying in between x=3.8 and 6 for flame I (corresponding to the smallest turbulent intensity), between 2.8 and 6 for flame II and between 1.6 and 6 for flame III (corresponding to the largest turbulent intensity). (Note that the "limiting" position x=6 is the position of the triple point in the laminar flame).

A plot of the mean distance to the inlet and its rms fluctuation versus the global turbulence intensity (Fig. 6 a) shows a monotonous relation. While fluctuations increase with turbulence, the mean position in the axis, or mean stabilization height, is smaller for higher turbulence. The turbulence level is thus favoring earlier combustion. This could seem to contradict experimental results in which the stabilization height of a flame in a jet is shown to increase with the Reynolds number of the jet. One should remark that while in a jet a higher Reynolds number implies both higher turbulence and higher mean inflow velocity, here only the turbulence level changes in the different simulations, while the mean inflow velocity remains constant. While the effect of a higher mean inflow velocity is that of increasing the lifting height, the effect of a stronger turbulence is to reduce it.

A first hint of the stabilization mechanism can be already obtained by analysis of Fig. 4 and of the instantaneous flame images such as those presented in Fig. 3. The flames appear to propagate towards the inlet initially from their laminar stable position (x=6), while maintaining a constant position in the y axis, slightly changed by turbulence driven convection. At some later time they find a local flow speed higher than their propagation speed. At this point they would propagate downstream and the flame would be eventually blown-off, if it was not for the reignition events triggered by occasional hot pockets detached from the hot gas layer by recirculation (or convected by recirculating large eddies in a gas turbine). When such an event occurs, a burning lean pocket is formed, which propagates towards richer mixtures and reignites a triple flame when it finds a stoichiometric mixture (that is, when it crosses the stoichiometric line). The trailing diffusion flame attached to the triple point joins then the receding triple flame, reuniting into a single flame again.

Figure 7 presents the computed axial fixedreference (u_f) and propagation (u_p) speeds of the most upstream triple point, together with the gas velocity u_g measured at the first and last triple point for flame II. A first observation is that, while the flame speed in the laboratory reference frame (u_f) is negative for important periods, which coincide with the periods in Fig. 4 in which the flame recedes, the flame propagation speed u_p is always positive. The imposed mean inflow speed U exceeds the flame propagation speed, and even if the flame modifies locally the flow, making it slower just upstream, the local gas velocity is most of the time higher than the propagation speed. Instantaneously, very high values of the propagation speeds are observed for both the first and the last triple points. When comparing this figure to Fig. 4 it is seen that these high propagation speed occurrences coincide for the first triple point with reiginition events, and therefore do not correspond to a true propagation of the flame. For the last triple point the peak velocities occur just after the reignition, when the flames merge. They are then special events of very high propagation speed produced by the extra amount of heat received from the triple flame upstream with which it merges. For the rest of the time, the local propagation velocity is about $2S_L$. In Fig. 8 the propagation speed for flames I, II and III is plotted with a scaling focused in the lower values, which eliminates the peaks corresponding to reignition. For the three flames the "true" local propagation speed, that is, the propagation speed away from reignition/merging events, is only slightly varying. Its mean value can be obtained by time averaging after discarding speed values corresponding to times where multiple triple points coexist, and for all the three simulations a mean value of about $2S_L$ is obtained, independently of the global turbulence intensity. Also plotted in Fig. 8 is the local gas velocity at the triple point, showing no correlation to the flame speed, as was found in [14] (the computed correlation is about 0.34). Figure 6 b and c present the computed mean propagation speed and its rms value for flames I,II and III and the computed "true" propagative mean and rms values, showing that whilst the total speed is correlated to the turbulence intensity, the true speed is not. It should be concluded that while the local propagation speed is independent on the turbulence, the reignition effects depend on the global turbulence level.

The distinction between "true" flame propagation speeds and speeds corresponding to reiginition, and their different correlations to the local and global turbulence level provide an answer to findings of [14], which observed the propagation speed to be independent on the local turbulence and on the large scales, but found important variations in its value which could not be explained. This can be explained if in their experiment as here the propagation speed is independent of the local or global turbulence but there is a stabilization mechanism, not linked to propagation, which depends on the global turbulence level. The stabilization picture proposed by Su et al. [13], in which large scale struc-

tures produce a recirculation of the flame tip within the jet could be such a mechanism. But if it is the large scale structures which stabilize the flame, a correlation should have been found between the passage of large structures and the flame propagation speed in the experimental results of [14]. An explanation could be that, like in the present configuration, the stabilization mechanism is not acting directly at the triple point but at rich or lean premixed regions, in which case no correlation exists between the structures producing stabilization and the flame tip location or propagation speed. This, of course, is an hypothesis which should be verified in further studies.

4. Conclusions

In this paper the dynamics of turbulent diffusion flame stabilization in turbulent flows by hot combustion products recirculation is studied using DNS. A simplified configuration in which turbulence with different intensity levels is injected at the inlet of a mixing layer of diluted methane and air was simulated, using a high order compact finite differences code. Initially a laminar diffusion flame is stabilized in the domain by a hot gas layer, used here to simulate hot combustion products recirculation.

Analysis of the results shows that the subsequent turbulent flames consist in unsteady distorted triple flames with propagation speed of about $2S_L$, driven downstream by the higher mean inflow speed imposed $U = 3.5S_L$. Occassional reignition events occur, which are responsible of stabilization of the otherwise blown-off flames. Both the mean and fluctuation of the flame position in the injection axis are found to depend on the turbulence level imposed. The mean and fluctuation of propagation speed seem to be also dependent on the turbulence level, but when artificially high non propagating events related to reignition of a new triple flame are eliminated, the computed mean and rms of the "true" propagation speed result independent of the turbulence level. This can explain recent measurements by Upanietks et al. [14], which in a diffusion flame stabilized in a jet found a strongly fluctuating flame propagation speed, but uncorrelated to local turbulence. The proposed stabilization mechanism is based on triple flames propagating at a nearly constant speed, independent of the local or global turbulence, and stabilized by occassional events driven by large scale structures, similar to the mechanism proposed by Su et al. [13].

Acknowledgements

Computing time was provided by IDRIS (Orsay, France).

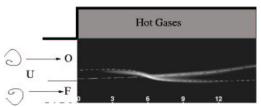


Fig. 1: Simulation configuration and initial laminar flame. A greyscale is used to represent reaction rate with white corresponding to its maximum. White lines represent the $T=T_i$ (short dash) and $Z=Z_{st}$ (long dash) isolines.

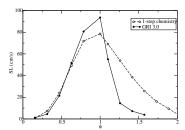
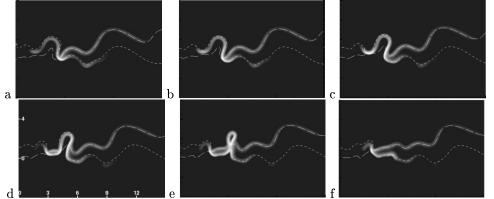


Fig. 2: Speeds of planar premixed flames with the 1-step chemistry and with GRI 3.0.

References

- Y. Mizobuchi, S. Tachibana, J. Shinjo, S. Ogawa, T. Takeno, Proc. Combust. Inst. 29 (2002), 2009-2015.
- [2] L. Vanquickenborne, A. van Tiggelen, Combust. Flame 10 (1966), 59–69
- [3] N. Peters, F.A. Williams, AIAA J. 21 (1983), 423–429.
- [4] A. Liñán, A. Crespo, Combust. Sci. Techno. 14 (1976) 95–117
- [5] A. Liñán, in Combustion in High Speed Flows (1994) Kluwer 461-476.
- [6] J.W. Dold, Combust. Flame 76 (1989) 71–88.
- [7] L. Muñiz, M.G. Mungal, Combust. Flame 111 (1997) 16-21.
- [8] D. Han, M.G. Mungal, Proc. Combust. Inst. 28 (2000) 537–543.
- [9] G.R. Ruetsch, L. Vervisch, A. Liñan, Phys. Fluids 7 (1995) 1447-1454.
- [10] V. Favier, L. Vervisch, Proc. Comb. Inst. 27 (1998), 1239-1245.
- [11] P. Domingo, L. Vervisch, J. Réveillon, Combust. Flame 140 (2005) 172–195.
- [12] E. Fernández-Tarrazo, M. Vera, A. Liñán, Combust. Flame in press (2005)
- [13] L.K. Su, O.S. Sun,M.G. Mungal, Combust. Flame in press (2005)
- [14] A. Upatnieks, J.F. Driscoll, Ch.C. Rasmussen, S.L. Ceccio, Combust. Flame 138 (2004) 259– 272.
- [15] A. Bourlioux, B. Cuenot, T. Poinsot, Combust. Flame 120 (1998) 143-159.
- [16] M. Baum, D. Haworth, T. Poinsot and N. Darabiha, J. Fluid Mech. 281 (1994) 1—32.
- [17] C. Jiménez, B. Cuenot, T. Poinsot Tech. Rep. TR CFD/01/47 (2001) available at www.cerfacs.fr.



d $\frac{3}{4}$ $\frac{6}{4}$ $\frac{9}{4}$ $\frac{12}{4}$ $\frac{12}{4}$

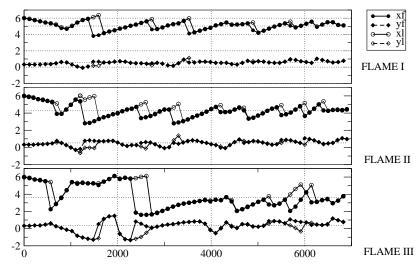


Fig. 4: Fluctuations in time of the position of the first triple point (xf,yf) and the last triple point (xl,yl).

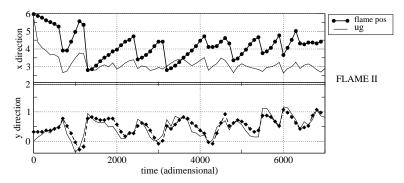
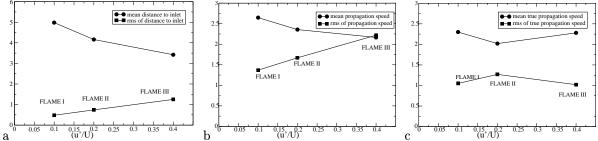


Fig. 5: Position of the triple point and gas velocity at the triple point u_g for flame II.



 $\frac{0.05}{0.1}$ $\frac{0.15}{0.15}$ $\frac{0.2}{0.25}$ $\frac{0.25}{0.3}$ $\frac{0.3}{0.35}$ $\frac{0.4}{0.4}$ $\frac{\sqrt{0}}{0}$ $\frac{0.05}{0.05}$ $\frac{0.1}{0.1}$ $\frac{0.15}{0.1}$ $\frac{0.25}{0.25}$ $\frac{0.3}{0.35}$ $\frac{0.35}{0.4}$ $\frac{0.05}{0}$ $\frac{0.05}{0.05}$ $\frac{0.1}{0.1}$ $\frac{0.15}{0.15}$ $\frac{0.25}{0.25}$ $\frac{0.25}{0.3}$ $\frac{0.35}{0.35}$ $\frac{0.4}{0.15}$ $\frac{0.05}{0.1}$ $\frac{0.05}{0.15}$ $\frac{0.15}{0.15}$ $\frac{0.25}{0.25}$ $\frac{0.25}{0.25}$ $\frac{0.3}{0.35}$ $\frac{0.35}{0.1}$ $\frac{0.3}{0.15}$ $\frac{0.4}{0.15}$ $\frac{0.05}{0.1}$ $\frac{0.15}{0.15}$ $\frac{0.25}{0.25}$ $\frac{0.25}{0.25}$ $\frac{0.3}{0.35}$ $\frac{0.35}{0.1}$ $\frac{0.4}{0.15}$ $\frac{0.05}{0.1}$ $\frac{0.15}{0.15}$ $\frac{0.25}{0.25}$ $\frac{0.25}{0.25}$ $\frac{0.3}{0.35}$ $\frac{0.35}{0.1}$ $\frac{0.35}{0.15}$ $\frac{0.4}{0.15}$ $\frac{0.05}{0.15}$ $\frac{0.1}{0.15}$ $\frac{0.15}{0.15}$ $\frac{0.25}{0.25}$ $\frac{0.25}{0.25}$ $\frac{0.3}{0.35}$ $\frac{0.35}{0.1}$ $\frac{0.35}{0.15}$ $\frac{0.1}{0.15}$ $\frac{0.15}{0.15}$ $\frac{$

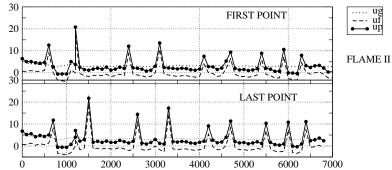


Fig. 7: Local flow velocity (ug), and fixed-frame (uf) and propagation (up) speeds at the first and last triple points for flame II.

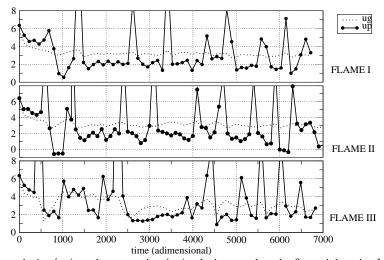


Fig. 8: Local flow velocity (ug), and propagation (up) velocity speed at the first triple point for flames I,II and III.