

Interactions between Mixing, Flame Propagation, and Ignition in Non-Premixed Turbulent Flames

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1 Introduction

Despite the awesome potential of diagnostic techniques to analyse the various physical mechanisms involved in turbulent combustion, their applications do not always satisfy the over-developed curiosity of physicists and modellers whose interest is often concentrated on their couplings at the smallest unresolved scales of the turbulent reactive flow. Moreover, depending on the configuration studied, the application of such diagnostics may be rather complex and can even become impossible under some aggressive environments. In this context, computational fluid dynamics (CFD) techniques appear as powerful complementary tools to experiments so as to conduct relevant physical analyses. However, the physical mechanisms involved in these turbulent reactive flows display such a wide range of characteristic scales that the statistical, i.e., Reynolds-averaged Navier-Stokes (RANS), representation or the filtered, i.e., large eddy simulation (LES), descriptions are still required to proceed with their numerical simulations. Accordingly, modelling strategies must be proposed to reproduce the effects of the unresolved mechanisms including turbulent transport and mixing between chemical species, heat release resulting from the unresolved production / destruction of chemical species as well as the associated propagation or auto-ignition phenomena. The mid-term objective of the present study is to take advantage of numerical simulations used in conjunction with diagnostic techniques applied on an experimental test rig, that has been recently designed to study non-premixed turbulent combustion at the PPRIME Institute of Poitiers. In the corresponding experimental setup the injection velocities of reactants can reach rather large values leading to flame lift-off from the burner rim. Partially premixed flame edges thus propagate towards the fresh reactants, stabilising the whole flame structure. The temperature of the oxidizing stream can be increased by vitiation with burned gases so as to promote flame stabilisation processes. This is presently obtained thanks to eight secondary burners delivering combustion products in a large coflowing stream. It is noteworthy that such a vitiation procedure is often retained in practical devices such as industrial boilers to limit temperature gradients and NO_x production of thermal origin [1]. Sufficiently large values of the vitiated air temperature may also trigger auto-ignition phenomena, see references [2, 3], thus leading to a competition between mixing, propagation, and auto-ignition mechanisms. Several jet-in-hot-coflow (JHC) burners have been recently designed to study the influence of preheating and dilution on stabilisation mechanisms [4, 5]. A shorter-term objective of this study is to develop a numerical simulation procedure as simple as possible to study the interactions between these various physical mechanisms. In the case of direct numerical simulations (DNS), a detailed chemical mechanism associated with the corresponding species transport equations may provide a satisfactory representation of species mixing, propagation and auto-ignition. However, the RANS and LES frameworks cannot deal with the strong non-linearity of the Arrhenius laws that drive the characteristic lengths

and times of the smallest scales of the flows. Therefore, with the objective of proposing a turbulent combustion model as simple as possible, we choose here to treat the different mechanisms separately, i.e., by using one single scalar variable dedicated to the description of each of them: a mixture fraction $\xi(x, t)$ to evaluate scalar mixing [6], a progress variable $c(x, t)$ to follow the flame propagation mechanism [7], a residence time to delineate the possible influence of auto-ignition processes [8, 9]. Then, we investigate their interactions. In practice, the use of such simple models does involve some modelling parameters: the corresponding numerical simulations cannot be considered as fully predictive so far. However, detailed sensitivity analyses of the computational parameters with respect to experimental data may lead to a clear delineation of their relevant range of variations. Moreover, the corresponding computational results may also be useful to optimize the design of the experimental setup or the choice of operating conditions, as well as measurement settings and postprocessing parameters. Accordingly, such a joint numerical-experimental study will allow to complement experimental data, leading to a solid understanding of the model behaviours associated to an accurate physical analysis of the competition between mixing processes, propagation and auto-ignition phenomena. The experimental setup and flow conditions are first presented in the next section. The combustion model is then briefly described and the first results commented in a third section. Eventually, the complementary results that will be presented at the conference are shortly summarised in a last section.

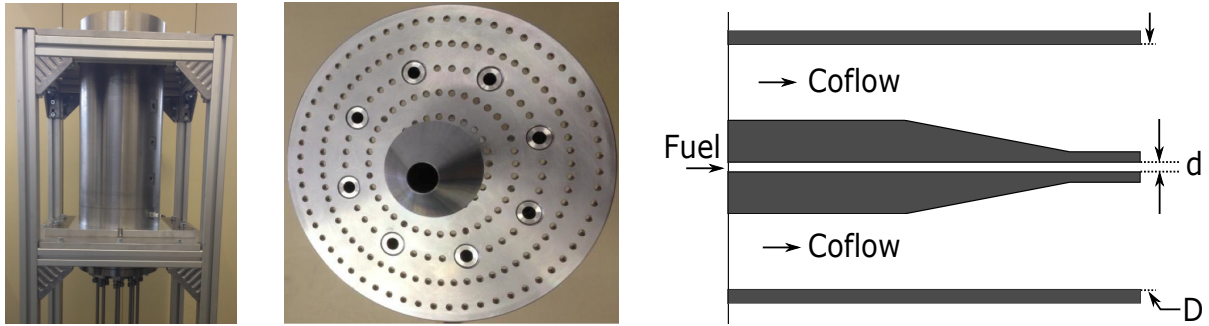


Figure 1: Left: global view of the *Demoxya* burner; Middle: central nozzle and coflowing injection plate; Right: details of the fuel injection

2 Experimental configuration and numerical setup

In this first step of the study, the simple turbulent combustion model implemented is not only applied to the numerical simulation of the experimental setup developed at PPRIME Institute but also to two other reference configurations: (i) a laboratory-scale burner that has been designed to study MILD (Moderate and Intense Low oxygen Dilution) combustion [10] and (ii) the burner designed by Cabra et al. [11, 12] to study flame stabilisation in hot environments. Turbulent non-premixed jet flames are analyzed in these three cases. Figure 1 displays the geometry of the *Demoxya* burner operated at the PPRIME Institute. The inner diameters of the central jet and coflow are $d = 8$ mm and $D = 210$ mm, respectively. The vitiation is obtained thanks to eight secondary burners and the temperature of the fuel jet is controlled thanks to water recirculation inside the central piece of metal that constitutes the inner nozzle, see the right side of Fig. 1. The experimental conditions considered in references [10, 11] are listed in Tables 1 and 2, respectively. In these tables, V denotes the bulk velocity, T is the temperature, and X_α is the mole fraction of species α . The detailed experimental conditions of the *Demoxya* burner are still being established. The study zone corresponds to heights ranging from $z = 0$ mm (nozzle exit plane) to $z = 100$ mm downstream of the injection nozzle. The computational model described in the next section has been implemented in the CFD solver *Code_Saturne* developed by EDF [13]. Turbulent mixing is represented through a standard one-point two equations $\tilde{k}$ - $\tilde{\epsilon}$ model. Unstructured two-dimensional

meshes featuring between 20,000 and 100,000 cells have been generated to represent a slice of the physical domain. The top side (resp. bottom side) of the computational domain corresponds to an outlet boundary condition (resp. an inlet boundary condition). For the largest mesh, the time required to obtain the full convergence of the numerical simulation is a few hours on a six-cores quadri-processors computer, and it is only a few minutes, once the initial conditions are well-established, on the smallest mesh. Such a small computational cost clearly offers one of the greatest advantages of this modelling framework. Moreover, we will see that the obtained results, to be presented in the next section, are in fairly satisfactory agreement with available experimental data. However, as further discussed below, the modelling proposals must be relevant to a wide range of turbulent combustion modes and regimes to reach such a level of agreement and the sensitivity to modelling parameters therefore deserves to be studied in detail.

Table 1: Operative conditions HM9% of reference [10]

	diameter (mm)	V (m/s)	T (K)	Y_{O_2}	Y_{N_2}	Y_{H_2O}	Y_{CO_2}	Y_{CH_4}	Y_{H_2}
Central jet	4.25	73.5	305	0	0	0	0	0.885	0.115
Coflowing jet	82	3.2	1300	0.09	0.79	0.065	0.055	0	0
Wind tunnel	-	3.2	300	0.233	0.767	0	0	0	0

Table 2: Operative conditions of Cabra et al. [11, 12]

	diameter (mm)	V (m/s)	T (K)	X_{O_2}	X_{N_2}	X_{H_2O}	X_{CH_4}	X_{H_2}
Central jet	4.57	100	320	0.15	0.52	0.0029	0.33	0
Coflowing jet	210	5.4	1,350	0.12	0.73	0.15	0.0003	0

3 Analysis of the turbulent combustion model behaviour

3.1 Mixture fraction variable

As the flow considered here is non-premixed, the primary mechanism that must be taken into account by the turbulent combustion model corresponds to the mixing processes. Transport equations are considered for the mixture fraction mean $\tilde{\xi}$ and variance $\tilde{\xi''^2}$, which are used in conjunction with tabulated chemistry. The corresponding tabulations are obtained from Cantera computations [14]. The left side of Fig. 2 displays the corresponding temperature profiles plotted versus the mixture fraction as obtained from either the chemical equilibrium or from strained laminar diffusion flamelets. As expected, significant differences can be observed between chemical equilibrium and strained diffusion flamelet results, which highlight the influence of both molecular diffusion and finite-rate chemistry effects. However, Fig. 2 also shows that the temperature profiles issued from strained diffusion flamelet computations remain similar whatever the value of the reference strain-rate, which has been evaluated from $\chi = (V_F + V_O)/L$, with V_F and V_O the fuel and oxidizer stream bulk-flow velocities and L the separation distance between the two injectors. Such a behaviour confirms that, despite the wide range of chemical characteristic time scales introduced through the consideration of a detailed chemical mechanism, the heat release can still be described - in a first approximation - through a single characteristic time scale. The largest temperature difference observed among these various opposed diffusion flame computations is less than five percents and is located around stoichiometry. Stoichiometric conditions are reached only within a very restricted part of the non-premixed turbulent flames simulated so that the consideration of any value of the strain-rate will only lead to small differences on the mean temperature field. In addition to this, our present objective is to perform a detailed sensitivity analysis of the numerical parameters that are known to be the most influential on numerical results. Therefore, we choose

to store chemical data computed for one single counter-flow diffusion flame with a given value of the strain-rate $\chi = 100 \text{ s}^{-1}$. Finally, the sole modelling parameter of the model is the scalar to turbulent time scale ratio $C_\xi = \tau_\xi / \tau_T$, which is used to fix the value of the mean scalar dissipation rate (SDR) value. For the sake of simplicity, the linear relaxation model $\tilde{\varepsilon}_\chi = \tilde{\xi}''^2 / (C_\xi \tau_T)$ is used with a standard value $C_\xi = 0.8$. In this respect, the resort to generalized closures such as the one studied in reference [8] may offer some perspectives for future works.

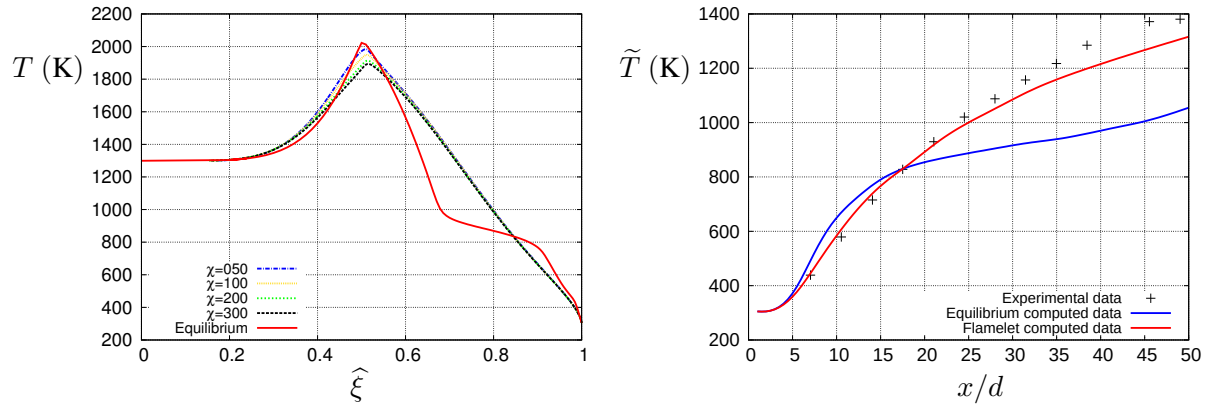


Figure 2: Left: temperature profiles for distinct values of the strain-rate χ plotted versus $\hat{\xi}$, a normalised mixture fraction as defined in reference [15]; Right: mean temperature axial profiles for the conditions of reference [10], computational results and experimental data.

In practice, the mean values of any quantity (density, temperature, etc.), as well as any-other relevant cross correlations [15], are stored for each possible values of the mean and normalized variance (i.e., segregation rate) of the mixture fraction. Figure 2 (right) compares the computed axial profile of the mean temperature with experimental data documented in reference [11]. The chemical equilibrium approximation underestimates significantly the mean temperature levels whereas diffusion flame computations are in rather satisfactory agreement with experimental data.

The above representation is suitable for turbulent non-premixed flames attached to the burner rim such as the one displayed on the left side of Fig. 3. However, to account for the possible occurrence of lifted flames, a generalized framework must be settled. In such situations, a premixture is indeed formed just downstream of the burner and partially premixed conditions must be considered. To keep pace with our initial objective of using a turbulent combustion model as simple as possible, only one additional table will be created and the corresponding data will be representative of the non-reactive mixing between the two streams. Accordingly, the strained diffusion flamelet table is representative of burned product states and the additional table will be representative of non-reactive states. To select the right table to be read within the course of the numerical simulation, a relevant progress variable must now be introduced.

3.2 Progress variable

A single progress variable $c(\mathbf{x}, t)$ is considered here; it is defined to be $c \equiv 0$ in fresh reactants and $c \equiv 1$ in fully burned combustion products. According to the previous section, tabulated laminar diffusion flamelets are considered as the elementary building blocks, i.e., the focus is on fast-chemistry regimes of turbulent combustion. The mean value of the progress variable thus provides the proportion of burned products. However, the cross correlation between the progress variable and the mixture fraction, which is required to precisely determine the composition of the partially premixed mixture is presently neglected for the sake of simplicity, i.e., $\widetilde{c''\xi''} = 0$. As a direct consequence, the mixture fraction PDF is the

same in either the fresh reactants or the fully burned products of combustion. This allows to use the two tables, which were discussed in the previous subsection, with the same inputs, i.e., the same values of the mean and variance of the mixture fraction. This assumption is only valid for characteristic time scales of the reactive processes that are sufficiently small compared to mixing time scales; it is thus expected to be justified when the flame propagates in near-stoichiometric fresh reactants. It is however expected to fail when the flame reaches extinction limits, i.e., in either very rich or very lean mixtures. The closure of the chemical source term in the transport equation of the mean progress variable must account for the intermittency that is associated to the flamelet regime of turbulent combustion. Here it is simply expressed by $\tilde{\omega}(\tilde{c}) = \alpha(1 - S)\tilde{c}(1 - \tilde{c})$, where the segregation-rate S includes a parameter β that needs to be adjusted to obtain the right velocity of propagation: $S = 1/(1 + \beta Da_T^{-1})$ with $Da_T = \tau_T/\tau_{chem}$ a Damköhler number. The value of α and τ_{chem} can be determined from the computation of laminar premixed flames [7], the latter being subsequently tabulated as a function of the mixture fraction. Figure 3 (left) displays the mean temperature field obtained from the numerical simulation of

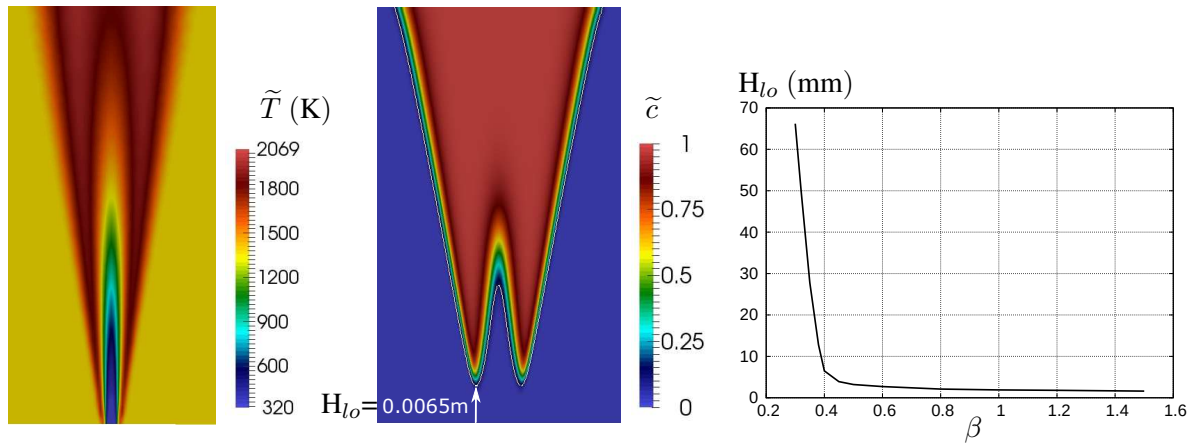


Figure 3: Left: temperature field obtained without consideration of the mean progress variable transport equation; Middle: mean progress variable field with iso- $\tilde{c}$ value $\tilde{c} = 0.1$ (white line); Right: lift-off height sensitivity to the value of the modelling parameter β .

the Cabra's experiment with the sole consideration of the transport equations for the mixture fraction mean and variance; the turbulent non-premixed flame is attached to the burner rim. Figure 3 (middle) reports a typical result obtained with the consideration of the mean progress variable transport; the flame is lifted off from the nozzle. Finally, a sensitivity analysis of the lift-off height H_{lo} to the value of the modelling parameter β has been performed. It is presented in Fig. 3 (right) and shows that the dependency to this modelling parameter is strongly non-linear.

4 Additional results and conclusions

The simple model introduced above allows to represent the competition between mixing and propagation processes occurring in non-premixed turbulent flames. The obtained results confirm that the consideration of tabulated chemistry based on strained diffusion flamelets may lead to a satisfactory representation of the turbulent flame. The strain-rate value is not found to affect the results significantly, thus confirming that one single tabulation can be sufficient. Finally, only one relevant modelling parameter has been clearly identified and its behaviour has been studied through a sensitivity analysis. A transport equation for a normalized residence time has been also considered to account for ignition phenomena but the corresponding results are not presented here for the sake of conciseness. The use of

this additional variable requires the introduction of one additional tabulation of chemical data and it introduces one supplementary modelling parameter. The corresponding variable will be used to study the competition between flame propagation and auto-ignition processes. The final objective is to apply the whole procedure to the computation of the new experimental set-up that is now available at the PPRIME Institute and to delineate the possible range of variation of the modelling parameters.

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