Relevance of Basic Turbulent Premixed Combustion Models for Accurate Simulations of V-shaped Flames

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1 Introduction

The development of computational fluid dynamics (CFD) tools over the last decades allows their today's applications to the numerical simulations of various industrial turbulent flows featuring complex geometries and realistic conditions. However, the physical phenomena involved in 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 Simulations (LES), description of these flows are still required to proceed with their numerical simulations. The direct numerical simulation of such flows indeed remains unrealisable in the very near future. The use of LES may provide a satisfactory description of the large-scale turbulent dynamics at the price of an *intermediate* computational cost but its practical engineering use still remains limited. Accordingly, RANS and U-RANS approaches still remain the reference tools to proceed with the industrial design of energy conversion devices. In practice, the resort to any of these two frameworks (i.e. RANS or LES) do involve the use of some numerical and modeling parameters so that the corresponding numerical simulations cannot be considered as fully predictive so far. Therefore, the models involved in these numerical simulations and their behaviors must be perfectly understood so as to obtain results that recover relevant trends and can be useful to complement experimental data. The objective of the present study is precisely to provide a detailed sensitivity investigation and analysis of such model behaviors when applied to the numerical simulation of a turbulent premixed V-shaped flame.

One specific difficulty associated with the numerical simulation of turbulent reactive flows lies in the domains of validity of the turbulent combustion models, which remain quite restricted. In a given reactive flow, the nature of the turbulent combustion regime is strongly variable from place to place, and this conclusion holds for flows of practical, i.e. industrial, interest as well as for simplified laboratory geometries. For instance, in the turbulent V-shaped flame studied herein, the main part of the flame brush can be described as belonging to the flamelet regime, which is characterized by infinitely small chemical time scales compared to characteristic turbulent time scales. However, on the one hand, the increase of turbulent kinetic energy downstream of the stabilization rod may lead to some thickening of the flame, and this part of the turbulent reactive flow just behind the rod could even be considered as a well-stirred reactor. On the other hand, in the fresh reactants, in front of the flame brush, the chemical time becomes infinitely larger than the characteristic turbulent time scales. Therefore, the turbulent combustion models proposed for the numerical simulation of such a reactive flowfield must be as simple as possible but must also be realistic enough to handle such a wide range of variations of the turbulent combustion regime. Here, we choose to analyze simple models, which are able to change their functional form inside the computational domain, depending on the turbulent combustion regime encountered. To account for these possible changes, a relevant criterion must be set forth and it is based here on algebraic expressions of the segregation rate.

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2 Computational domain and numerical setup

The retained numerical setup is representative of the experimental configuration studied by Degardin *et al.* [1, 2]. The turbulent flames are stabilized on a 0.8 mm diameter heated rod placed downtream of a vertical wind tunnel of 80×80 mm^2 square section. The combustion chamber is fed by an air flow rate of 86 Nm^3/h. Mixtures featuring different stoichiometries can be otained and it is also possible to produce an upstream stratified flow with a transversal gradient of equivalence ratio. The turbulence is generated from grids located 70 mm before the stabilizing rod location (i.e. z=0). The study zone corresponds to heights ranging from z=90 mm to z=170 mm downstream of the turbulence generating grid. In this zone, the velocity field has been characterized from particle image velocimetry (PIV) cross-correlation technique. A method based on the simultaneous measurements of temperature and fuel mole fraction by Rayleigh scattering and acetone planar Laser-induced fluorescence (PLIF) signals is used to evaluate the temperature and mixture fraction fields. Further details can be found in references [1, 2]. The

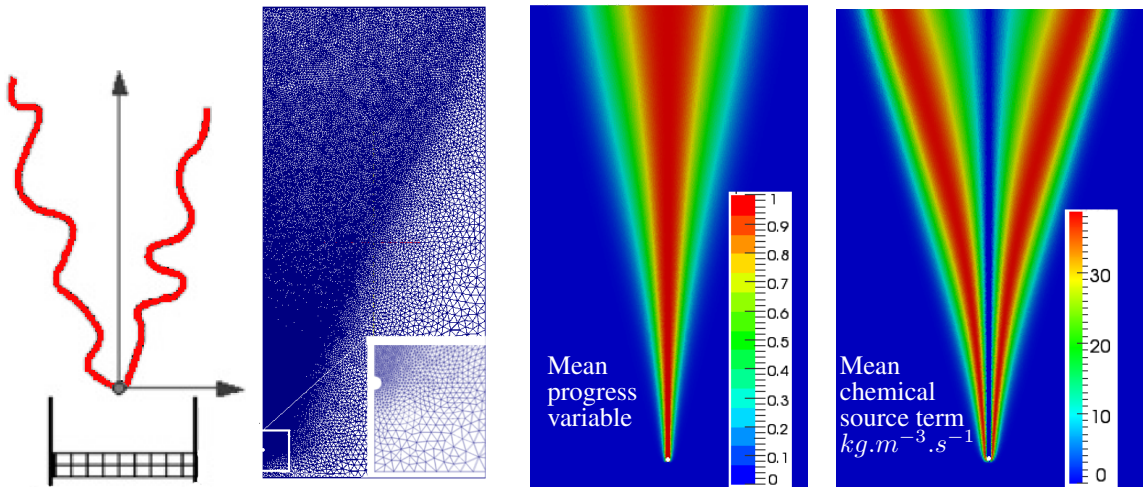

Figure 1: Sketch of the turbulent V-shaped flame, the corresponding computational domain and the field of mean progress variable and mean chemical source term

model described in the next sections has been implemented in the CFD solver *Code-Saturne* developed by EDF [3]. Turbulent mixing is represented through a standard one-point two equations k-ϵ model. Experimental results obtained in non-reactive conditions are used to settle inlet boundary conditions so as to reproduce correctly the grid turbulence decay following the procedure described in reference [2]. The corresponding inlet conditions for the velocity field are: $\widetilde{U}$=3.2 m/s, $\widetilde{V}$=0 m/s, $\widetilde{k}$=0.12 m^2/s^2, $\widetilde{\epsilon}$=10 m^2/s^3. An unstructured two-dimensional mesh featuring approximately 50,000 cells has been generated to represent half of the physical domain. The corresponding mesh is depicted in Fig.(1). The top side (respectively bottom side) of the computational domain corresponds to an outlet boundary condition (respectively an inlet boundary condition). From a numerical point of view, combustion has been stabilized through the use of an additional source term [1] that applies in computational cells neighboring the heated rod. The influence of this ignition procedure will be discussed later on. The time required to obtain the full convergence of the numerical simulations is approximately two hours on a single node bi-processors computer and approximately fifteen minutes once the initial conditions are well established. We expect that it will be possible to run such numerical simulations on an performant smartphone in the very near future and, from a practical point of view, the cheapness of such computational tools clearly offers one of its greatest advantages. Moreover the obtained results, to be presented in the next section, are in fairly good agreement with experimental data. However, as further discussed below, the modeling proposals

[1] This is a chemical progress variable source term.

must be relevant to a wide range of turbulent combustion regimes to reach such a level of agreement and the sensitivity to modeling parameters therefore deserves to be studied in details.

3 Turbulent combustion modeling

In this study, a unique progress variable $c(\boldsymbol{x},t)$, defined to be $c\equiv 0$ in the fresh unburned mixture and $c\equiv 1$ in combustion products, is considered. Accordingly, Lewis numbers for all species are close to unity, and heat losses as well as composition inhomogeneities are not addressed. Thus, the Favre averaged progress variable $\widetilde{c}=c-c''$ is solution of the following balance equation:

$$\frac{\partial\overline{\rho}\widetilde{c}}{\partial t}+\frac{\partial}{\partial x_k}(\overline{\rho}\widetilde{u_k}\widetilde{c})+\frac{\partial}{\partial x_k}\left(\overline{\rho u_k''c''}\right)-\overline{\frac{\partial}{\partial x_k}\left(\rho D\frac{\partial c}{\partial x_k}\right)}=\overline{\omega(c)}, \tag{1}$$

where u_k denotes the velocity field, $\rho(c)$ the density of the mixture, D the coefficient of molecular diffusion and $\omega(c)$ is the chemical reaction rate.

As it is well known, the closure of the mean chemical rate $\overline{\omega(c)}$ appearing in Eq.(1) is one of the most important sub-problems in the field of turbulent combustion modeling. A closed expression for this term can be obtained by using modeling assumptions that depend on the regime of turbulent combustion under consideration. This challenging problem may be simplified to a tractable form provided that one assumes the local reaction zones to remain sufficiently thin compared to fluid dynamics characteristic length scales (Kolmogorov length scale). The flame front thus appears as an interface separating fresh reactants from fully burnt gases and it may be described as a geometrical entity. Many *geometrical formalisms* have been proposed to deal with such a picture of turbulent premixed flames. Some are based on a field equation (G-field transport equation), as introduced by Williams [4], while others rely on the flame surface density (FSD) concept or on flame wrinkling descriptions. Others strategies incorporate the influence of unresolved scalar fluctuations thanks to *statistical approaches* often through the consideration of one-point one-time probability density functions [5] or at the level of a conditional moment closure. Finally, for sufficiently large values of the Damköhler number Da_T, the mean burning rate becomes limited by turbulent mixing quantified in terms of *scalar dissipation rate* values. Moreover, in reactive flows of premixed reactants at large Damköhler and turbulence Reynolds numbers, i.e. Da_T and Re_T, the flamelet regime of turbulent combustion applies and it is well known that the mean scalar dissipation rate (SDR) and mean reaction rate $\overline{\omega(c)}$ are inter related, see for instance references [6–8].
All these strategies require the use of transport equations for the flame surface density, the scalar dissipation rate or second order moments. However, these new equations involved many additional modeling parameters that are very difficult to set and that often must be adapted to the flow configuration considered. Therefore, results obtained with such strategies still cannot be retained for practical predictive use. Therefore it is chosen here to focus on simpler algebraic expressions for the mean chemical rate itself, without solving additional transport equations. Thus, the challenge is now to propose simple closures, which apply for a wide range of turbulent combustion regimes and do involve only the smallest possible number of relevant modeling parameters.
The simplest and early closure proposed to deal with turbulent reactive flows of premixed reactants corresponds to the eddy break-up (EBU) approach [9], it writes :

$$\overline{\omega(c)}_{EBU}=\overline{\rho}C_1\widetilde{c}(1-\widetilde{c})/\tau_t \tag{2}$$

where the EBU constant is C_1 and the characteristic turbulent time scale is $\tau_t=k/\epsilon$ with k the turbulence kinetic energy and ϵ its dissipation rate. Figure 2 reports progress variable profiles obtained from experiments together with numerical simulations results issued from this closure applied with different possible values of the eddy break-up constant. It is observed that, for a given value of the eddy break-up constant, satisfactory results can be obtained but not simultaneously at both distances downstream of

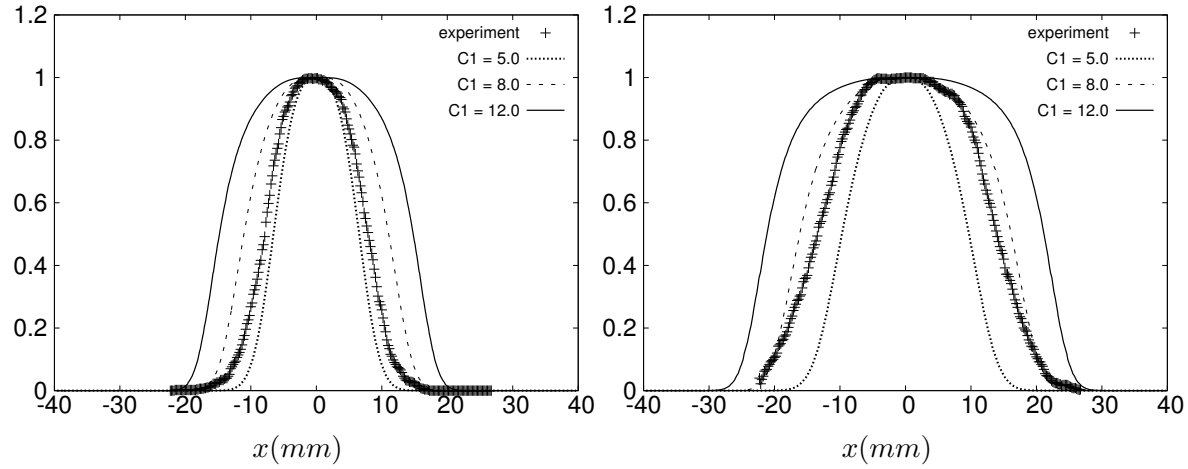

Figure 2: Progress variable profiles obtained from experiments and numerical simulations results at two different distances from the stabilization rod $z = 42.5mm$ (left) and $z = 70mm$ (left) for different values of the parameter involved in the mean chemical rate of Equation (2)

the stabilization rod, which confirms that the eddy break-up parameter C_1 cannot be considered as a constant.

The second algebraic closure studied here is the one proposed by Bray and his co-workers, see for instance [10]. It is hereafter denoted by $\overline{\omega(c)}_{BCL}$ and involves the segregation rate level S:

$$\overline{\omega(c)}_{BCL} = \overline{\rho}\widetilde{c}(1-\widetilde{c})(1-S)I_\omega/(I_1 - I_2) \tag{3}$$

where I_ω, I_1 and I_2 are constants that can be evaluated from laminar flame characteristics. The segregation rate is defined from the second order moment as follows: $S = \widetilde{c''^2}/(\widetilde{c}(1-\widetilde{c}))$ but it is chosen here to consider the segregation rate value as a constant input instead of solving an additional transport equation for the variance $\widetilde{c''^2}$. Thus, Eqs.(2) and (3) are very similar. However, the former does involve the integral turbulent characteristic time scale τ_t, which displays significant variations within the computational domain, while the latter does involve a chemical time I_ω, which is constant since it depends only on the characteristics of the fresh mixture, which is homogeneous since perfectly premixed in the present conditions. Figure 3 displays the progress variable profiles issued from experiments and from numerical simulations conducted by using the above closure with various values of the segregation rate. It is observed that, for a given value of the segregation rate S, satisfactory results can be obtained simultaneously at both distances downstream of the stabilization rod. Therefore, these results confirm that the segregation rate is a suitable parameter to characterize turbulent combustion. However, computational results are very sensitive to the choice of its value so that one may expect that it should be customized from one flow configuration to another. Furthermore, to take into account of the possible variations of the combustion regime within the flow, the segregation rate should be permitted to vary in the computational domain. Thus, in the next section, different analytical expressions are proposed for the segregation rate.

In the case of small values of the segregation rate, the turbulent combustion regime will no longer be the flamelet regime. The expression of the mean chemical rate must be designed to tend to $\overline{\omega(c)}_{BCLS}$, i.e. Eq.(3), when $S \to 1$, and to tend to the classical Arrhenius law $\overline{\omega(c)}_{Arr}$ when $S \to 0$. The simplest way to obtain such a behavior is to use the following linear bridging function:

$$\overline{\omega(c)} = (1-S)\overline{\omega(c)}_{Arr} + S\overline{\omega(c)}_{BCL} \tag{4}$$

This type of algebraic expressions have already been successfully used for the scalar dissipation rate [11, 12]. The same form may be also used to represent the scalar turbulent fluxes $\overline{\rho u_k'' c''}$ to address

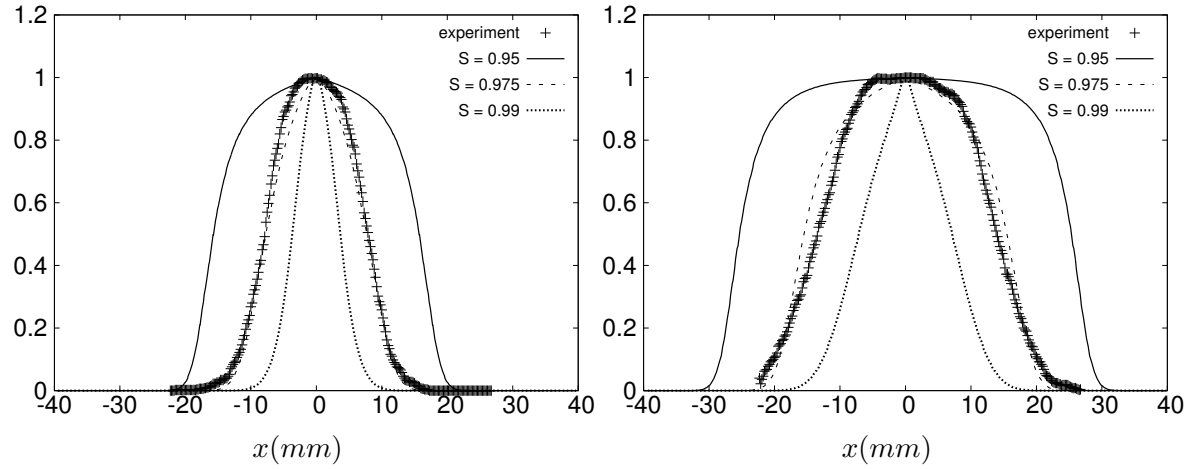

Figure 3: Progress variable profiles obtained from experiments and numerical simulations results at two different distances from the stabilization rod $z = 42.5mm$ (left) and $z = 70mm$ (right) for different values of the parameter involved in the mean chemical rate of Equation (3)

counter gradient diffusion in the flamelet regime. Both closures for the mean chemical rate and scalar turbulent fluxes are expected to be crucial to be able to recover the right propagation velocity of the turbulent flame brush. In particular, the recent work of Sabel'nikov and Lipatnikov [13] undoubtedly evidences the influence of these closures on the transition from pulled to pushed premixed turbulent flames.

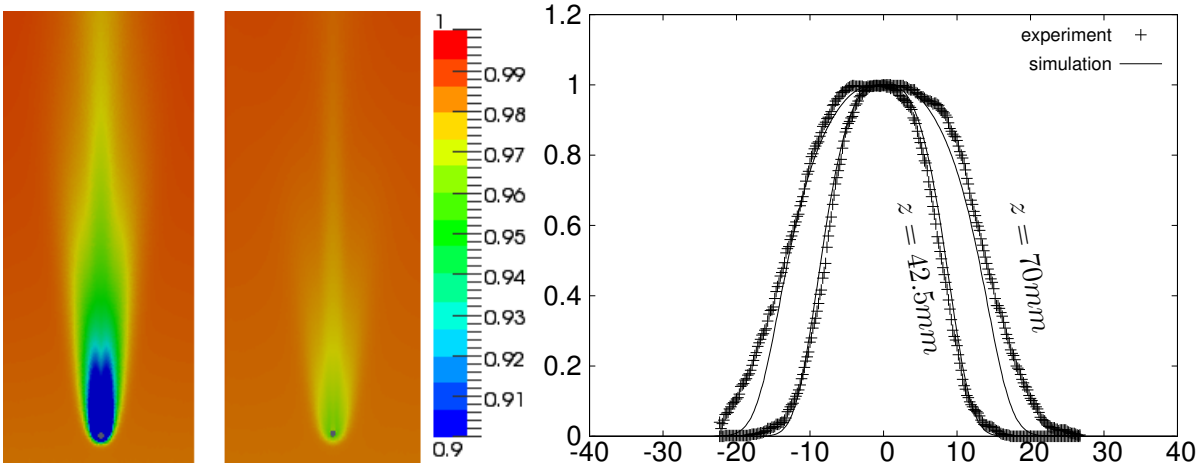

Figure 4: Fields of segregation rate obtained from Equation (5) (left) and (6) (middle) and progress variable profiles at two different distances from the stabilization rod (right)

4 Algebraic relations for the segregation rate and conclusions

The segregation rate must tend to unity when the chemical time τ_c becomes vanishingly small in comparison with the turbulent time τ_t, and conversely it must become vanishingly small when $\tau_t << \tau_c$. Thus, the first empirical expression proposed for the segregation rate is:

$$S = 1/(1 + C_2\tau_c/\tau_t), \tag{5}$$

where C_2 is a modeling parameter. It must be noticed that this expression makes Eq.(3) strictly equivalent to Eq.(2), i.e. EBU model, when $\tau_c << \tau_t$. In this limit case, the EBU constant is $C_1 = C_2\tau_c I_\omega/(I_1 - I_2)$. However, just behind the stabilizing rod, i.e. where the turbulent time τ_t decreases, Eq.(2) and Eq.(3) are no longer equivalent.

Another algebraic expression for the segregation rate is now proposed. It has been obtained from an asymptotic study conducted in the limit of infinitely large values of the Zel'dovich number, the details of which are not reported here just for the sake of conciseness. The obtained expression writes:

$$S = 1 - C_3 \exp\left(-\frac{1}{\sqrt{Ka}}\right), \tag{6}$$

where the Karlovitz number Ka is defined by $Ka = \tau_c/\tau_{\eta_K}$ with τ_{η_K} the Kolmogorov time scale and C_3 is a modeling constant.
Eventually, Figure 4 displays the fields of the segregation rate as obtained from the numerical simulations conducted with these two algebraic expressions, i.e. Eqs. (5) and (6). The progress variable profiles obtained using Eq. (5) are also reported and display a fairly good level of agreement with available experimental data. Further numerical results including a detailed sensitivity analysis of the different parameters will be presented in the extended abstract.

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