ANALYSIS OF ALGEBRAIC CLOSURES FOR THE TRANSPORT EQUATION OF THE MEAN PROGRESS VARIABLE APPLIED TO STAGNATING TURBULENT FLAMES

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Abstract
In the turbulent premixed reactive flows considered in this study, i.e. large Damköhler and Reynolds numbers, the flamelet regime of turbulent combustion applies and the scalar dissipation rate and mean reaction rate are inter related. In this situation various algebraic models for the mean chemical rate that are obtained from an equilibrium of the dominant terms of the transport equation for the scalar dissipation rate, are evaluated through their application to flames stabilized in a turbulent stagnating flow. An asymptotic analysis is first performed and results obtained through the resulting one-dimensional calculation are compared with the experimental data of Li et al. [1]. Eventually, three-dimensional CFD calculations including suited algebraic closures to represent the turbulent transport terms are carried out. Results are satisfactorilly compared to the experimental data of Cho et al. [2].

Introduction

In this work we describe premixed turbulent combustion in terms of a unique progress variable $c(x_k, t)$, with $c = 0$ in the fresh unburned mixture and $c = 1$ in combustion products. Thus, c is solution of the following balance equation

$$\frac{\partial \rho c}{\partial t} + \frac{\partial}{\partial x_k}\left(\rho u_k c\right) - \frac{\partial}{\partial x_k}\left(\rho D \frac{\partial c}{\partial x_k}\right) = \omega(c), \tag{1}$$

where u_k is the velocity field, $\rho(c)$ the density of the mixture, D the coefficient of molecular diffusion and $\omega(c)$ is the chemical reaction rate. In both frameworks of *RANS* or *LES* approaches to solve turbulent reacting flows an averaged balance equation for the progress variable must be solved. Following Eq.(1), such an averaged equation is written as:

$$\frac{\partial \overline{\rho}\widetilde{c}}{\partial t} + \frac{\partial}{\partial x_k}(\overline{\rho}\widetilde{u_k}\widetilde{c}) + \frac{\partial}{\partial x_k}\left(\overline{\rho u_k'' c''}\right) - \overline{\frac{\partial}{\partial x_k}\left(\rho D \frac{\partial c}{\partial x_k}\right)} = \overline{\omega(c)}, \tag{2}$$

where $c = \widetilde{c} + c''$ and the Favre averaged progress variable $\widetilde{c} = \overline{\rho c}/\overline{\rho}$ has been introduced.

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 subproblems 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. In the present contribution we take advantage of recent advances made in the modeling of the scalar dissipation rate:

$$\overline{\rho}\widetilde{\varepsilon}_c = \overline{\rho D \frac{\partial c''}{\partial x_k}\frac{\partial c''}{\partial x_k}},$$

see for example [3] [4] [5] [6], to analyze the problem raised by the numerical prediction of the mean reaction rate in a premixed turbulent flame. As it has been well known since the pioneering work of Bray [7], in reactive flows at large Damköhler and Reynolds numbers, the flamelet regime of turbulent combustion applies and the scalar dissipation rate and mean reaction rate are inter related through

$$\overline{\omega(c)} = 2\overline{\rho}\widetilde{\varepsilon}_c/(2c_m - 1), \tag{3}$$

where c_m is a constant parameter depending only on the statistical distribution of c through an individual flamelet, whose value lies in the range $0.7 - 0.8$. This relationship implies that, in the limiting case of infinitely large Damköhler number, molecular dissipation of the small scale fluctuations is controlled by chemistry. Accordingly a closed equation for the scalar dissipation rate can be used together with the system of equations for the mean velocity and progress variable fields as in the early proposal made by Borghi and Dutoya [8]. A more simple strategy is to consider an algebraic closure for the scalar dissipation rate. The simplest closure for this quantity is the classical relaxation model that writes:

$$\widetilde{\varepsilon}_c = C_B\widetilde{c''^2}\widetilde{\varepsilon}/\widetilde{k}. \tag{4}$$

Provided that some similarities exist between the scalar and velocity spectra, this model is often retained to represent the dissipation of a passive scalar. For reactive scalar, different algebraic closures have been proposed, see for example [9] [10] [11] [12][13], by considering an equilibrium between the dominant terms of the transport equation for $\widetilde{\varepsilon}_c$.

Here we apply this strategy to stagnating turbulent flame situations where the flame can be considered as an ensemble of laminar like local flamelets. In a first step an asymptotic analysis of the corresponding one-dimensional reacting flow is performed. Then, results from a full three-dimensional numerical simulation of the balance equations for the various flow quantities are given and discussed.

Asymptotic Analysis : description of the mean scalar equation

Stagnating turbulent premixed flames have been extensively used to analyze and validate closure models for turbulent reacting flows at large Damköhler number and relatively small incoming turbulence intensity. In such a geometry (see Fig. 1-a) the turbulent flame is stabilized in a stagnating flow formed by impinging a uniform stream of premixed reactants onto a solid planar surface. These studies were made possible thanks to a relatively simple similarity and asymptotic analysis of these reacting flows as well as the existence of a large set of experimental data involving a wide range of values for the mean flow induced strain rate, a quantity directly related to the positioning of the flame brush in the flow [1] [14]. The main objectives of the asymptotic studies were to assess models for the mean velocity field [15], for turbulent transports of mass and momentum [16], and eventually for the mean chemical rate $\overline{\omega(c)}$. As shown by Bray et al. [15], in the flamelet regime of turbulent combustion and under the assumption of small intensity incoming turbulence and large Reynolds number, the equation for the mean combustion progress variable in a stagnating turbulent flow can be written as:

$$\left(RW - \delta\frac{N_B}{2}(1 - 2\widetilde{c})\right)\widetilde{c}' = D_T(Z)\frac{(1+\tau)\widetilde{c}(1-\widetilde{c})}{(1+\tau\widetilde{c})^2} \tag{5}$$

where $()'$denotes differentiation with recpect to the axial non-dimensional coordinate $Z = z/d$ and d is the distance between the injection plane and the solid wall. R and W are the dimensionless mean density field and axial velocity respectively defined along the axis of the flow as

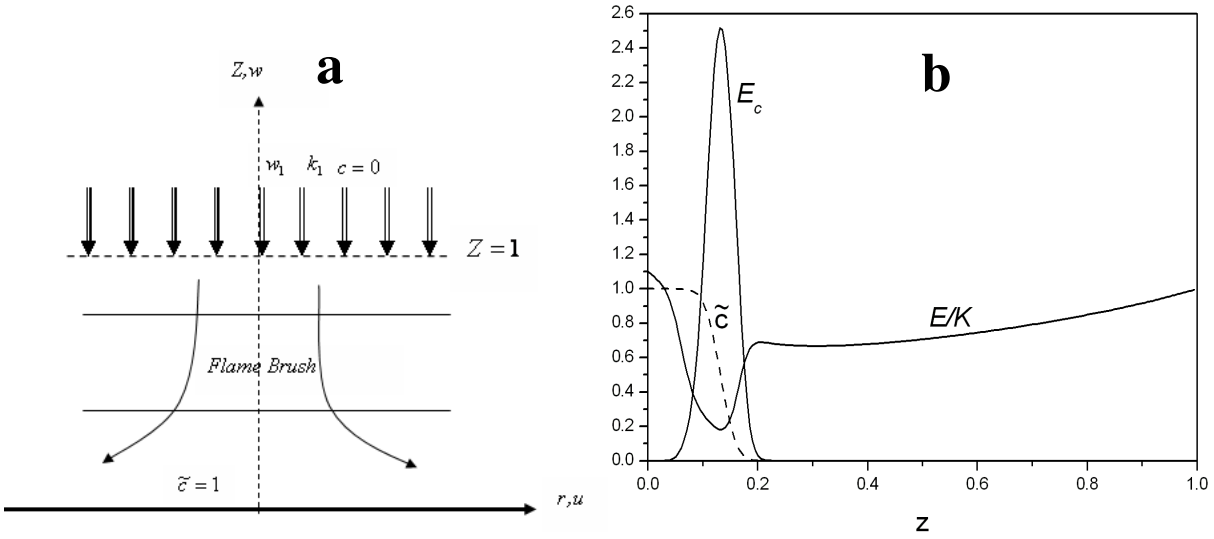

Figure 1: **a**: Schematic of the stagnating turbulent flame, **b**: mean structure of the flame brush corresponding to the Li et al. experiment [1]

[15]:

$$R(Z) = \overline{\rho}/\rho_1 \quad ; \quad W(Z) = \widetilde{w}(r, Z)/w_1 \tag{6}$$

where $\widetilde{w}$ is the axial component of the mean velocity field, and the subscript 1 denotes quantities taken at the exit plane $Z = 1$. The dimensionless mean density R is related to $\widetilde{c}$ through the equation of state, namely

$$R(1 + \tau\widetilde{c}) = 1 \tag{7}$$

where $\tau = \rho_1/\rho_0 - 1$ is the expansion factor. The subscript 0 denotes quantities taken at the plane $Z = 0$.

In Eq. (5) the second term of the left hand side represents turbulent transport of the progress variable [17]. This introduces (i) the Bray number $N_B = \tau S_l/k_1^{1/2}$ where S_l and δ_l are laminar flamelet velocity and thickness respectively, and (ii) the intensity of the incoming turbulence $\delta = k_1/w_1^2$. The RHS of Eq. (5) is proportional to the turbulent Damköhler number D_T, a function of the turbulent time scale associated to the scalar c, and whose form as a function of Z is still unknown at this point. In the closure system that we are considering in the present work D_T can be related to the scalar dissipation rate by using Eqs. (3) and (5). This yields

$$D_T(Z) = \frac{2(1 + \tau\widetilde{c})}{(2c_m - 1)(1 + \tau)\widetilde{c}(1 - \widetilde{c})} E_c(Z) \tag{8}$$

where we have introduced the dimensionless dissipation rate E_c defined as:

$$E_c(Z) = \widetilde{\varepsilon}_c(r, Z)\ d/w_1 \tag{9}$$

We now proceed by using the following strategy: for a given experiment a function $D_{T,\exp}(\widetilde{c})$ can be determined through Eq. (5) i.e. knowing R , W , $\widetilde{c}\,'$ from the experimental data. $D_{T,\exp}(\widetilde{c})$ can then be compared with the calculated $D_T(\widetilde{c})$ obtained from Eq. (8) provided $E_c(Z)$ can be determined through an equation, either differential or algebraic. However, at

large Damköhler and Reynolds numbers it has been shown (see for example [6]) that the balance equation for scalar dissipation E_c may often be reduced to an equilibrium between its leading production terms. This results in an algebraic form for the mean scalar dissipation rate, function of the turbulence time scale $\widetilde{\varepsilon}/\widetilde{k}$ and various parameters characteristic of both the turbulent flow and local flamelets. A general form for E_c can be written as:

$$E_c(Z) = F(\tau, N_B, Da; Z) \tag{10}$$

In Eq. (10) $Da = S_l d/\delta_l w_1$ is the Damköhler number associated to the geometry of the mean flow field and $K = \widetilde{k}/k_1,\ E = d\widetilde{\varepsilon}/w_1 k_1$ are the scaled turbulent kinetic energy and its dissipation rate respectively. Such algebraic models have been derived in particular by Borghi and his coworkers [12][13], Bray and Swaminathan [9], Kuan et al. [10], and Kolla et al. [11]. Therefore these models can be used in Eq. (8) to predict numerically the evolution of D_T through the flame brush, and comparisons can be drawn between experimental data provided by Li et al. [1] and numerical data issued from the various models.

The model of Bray and Swaminathan [9]

From an order of magnitude analysis of the various production terms appearing in the balance equation for the scalar dissipation rate $\widetilde{\varepsilon}_c$, Bray and Swaminathan have deduced the following expression for the scalar dissipation rate [9]:

$$\widetilde{\varepsilon}_c = \left(1 + \frac{2}{3} C_{\varepsilon c} \frac{S_l}{\widetilde{k}^{1/2}}\right) \left(C_{B1} \frac{S_l}{\delta_l} + C_{B2} \frac{\widetilde{\varepsilon}}{\widetilde{k}}\right) \widetilde{c}(1 - \widetilde{c}) \tag{11}$$

where S_l and δ_l are the laminar flame burning velocity and thickness respectively. As proposed in [9], the values of the three constant are $C_{\varepsilon c} = 0.1$, $C_{B1} = 0.24$, $C_{B2} = 0.21$. Using now the formalism set forth in the previous section for the stagnating turbulent flame, i.e. Eq. (9), Eq. (11) can be re written as:

$$E_c(Z) = \left(1 + \frac{2}{3} C_{\varepsilon c} \frac{N_B}{\tau K^{1/2}}\right) \left(C_{B1} D_a + C_{B2} \frac{E}{K}\right) \widetilde{c}(1 - \widetilde{c}) \tag{12}$$

where the flamelet assumption has been used to express the variance of the progress variable, namely $\widetilde{c''^2} = \widetilde{c}(1 - \widetilde{c})$.

The model of Kuan et al. [10]

The analysis made by Kuan et al. [10] leads to the following expression for the scalar dissipation rate:

$$\widetilde{\varepsilon}_c = \frac{C_\phi}{4} \left(1 + C_\phi^*(1 + \tau\widetilde{c}) S_l \frac{R_T^{1/4}}{\widetilde{k}^{1/2}}\right) \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{c}(1 - \widetilde{c}) \tag{13}$$

This expression depends *inter alia* on the Kolmogorov turbulent velocity scale, i.e. $u_K = \widetilde{k}^{1/2} R_T^{-1/4}$, where $R_T = \widetilde{k}^2/\nu\widetilde{\varepsilon}$ is the turbulent Reynolds number. We follow Kuan et al. [10] and use $C_\phi = 4$ and $C_\phi^* = 1.2$. Using again the formalism introduced to describe turbulent stagnating flames leads to:

$$E_c(Z) = \frac{C_\phi}{4} \left(1 + C_\phi^*(1 + \tau\widetilde{c}) N_B \frac{R_T^{1/4}}{\tau K^{1/2}}\right) \frac{E}{K} \widetilde{c}(1 - \widetilde{c}) \tag{14}$$

The model of Kolla et al. [11]

A further algebraic model for the scalar dissipation rate has been recently derived by Kolla et al. [11], from a detailled analysis of the full balance equation for this quantity. In this model the dissipation scalar rate is written as:

$$\widetilde{\varepsilon}_c = \frac{1}{\beta}\left((2K_c^* - \tau C_4)\frac{S_l}{\delta_l} + C_3\frac{\widetilde{\varepsilon}}{\widetilde{k}}\right)\widetilde{c}(1-\widetilde{c}) \tag{15}$$

or using the turbulent stagnating flames formalism:

$$E_c(Z) = \frac{1}{\beta}\left((2K_c^* - \tau C_4)D_a + C_3\frac{E}{K}\right)\widetilde{c}(1-\widetilde{c}) \tag{16}$$

where the various constants take the following values: $\beta = 10$, $K_c^* = 0.8\tau$, $C_3 = 1.5K_{al}^{1/2}/(1+K_{al}^{1/2})$, $C_4 = 1.1/(1+K_{al})^{0.4}$. $K_{al} \sim \delta_l/\tau_K S_l$ is the Karlovitz number, calling τ_K the Kolmogorov time scale $\tau_K = R_T^{-1/2}\widetilde{k}/\widetilde{\varepsilon}$.

The model of Borghi and coworkers [12][13]

The model proposed by Borghi and his coworkers is also deduced from an order of magnitude analysis of the production terms appearing in the RHS of the balance equation for the scalar mean dissipation rate, followed by proposals for the closure of the dominant contributions [12][13]. The final expression for the scalar mean dissipation rate is given by:

$$\widetilde{\varepsilon}_c = \left(1 + \frac{3}{2}C_{\varepsilon c}\frac{S_l}{\widetilde{k}^{1/2}}\right)\frac{A_1}{\beta}\frac{\widetilde{\varepsilon}}{\widetilde{k}}\widetilde{c}(1-\widetilde{c}) \tag{17}$$

Using the scaling introduced for the stagnating flame geometry leads to:

$$E_c(Z) = \left(1 + \frac{3}{2}C_{\varepsilon c}\frac{N_B}{\tau K^{1/2}}\right)\frac{A_1}{\beta}\frac{E}{K}\widetilde{c}(1-\widetilde{c}) \tag{18}$$

where A_1, β and $C_{\varepsilon c}$ are model constants. In the calculation relative to the turbulent stagnating flame we also retain $C_{\varepsilon c} = 0.1$, and the ratio A_1/β is adjusted so that the value $E_c(\widetilde{c} = 0)$ is similar to the one given by the other models.

Transport equation for the mean scalar dissipation rate

An alternative to the algebraic models described in the previous sections is to use a transport equation for the scalar mean dissipation rate. Restricting here ourselves to the case of stagnating turbulent flames exposed above, and using the Borghi and coworkers [12][13] closure model to express the leading production terms, such an equation for $E_c(Z)$ can be written as:

$$WE_c' = -\frac{\beta}{\left[1 + \frac{3}{2}C_{\varepsilon c}N_B/(\tau K^{1/2})\right]}\frac{E_c^2}{\widetilde{c}(1-\widetilde{c})} + A_1\frac{E}{K}E_c \tag{19}$$

where W is the axial velocity component defined earlier. In agreement with the asymptotic analysis used to solve the equations for the turbulent stagnating flame, i.e. vanishingly small turbulence intensity δ , turbulent transport is absent from this equation. This equation can be solved once the velocity field $W(Z)$, the progress variable field $\widetilde{c}(Z)$ and the turbulent time scale $E/K(Z)$ corresponding to the experimental data provided by Li et al. [1] are known (see

Bray et al. [16]). To avoid singularities on both reactants and burned products sides, a solution to this equation is sought in the form $E_c = \widetilde{c}(1-\widetilde{c})G(Z)$. Using Eqs. (5) and (8) this procedure results in the following equation for G :

$$WG' = G^2 \left[\frac{2\widetilde{c}-1}{c_m - 1/2} - \frac{\beta}{\left[1 + \frac{3}{2} C_{\varepsilon c} N_B/(\tau K^{1/2})\right]} \right] + A_1 \frac{E}{K} G \tag{20}$$

As $W(Z=0) = 0$, the boundary condition to be used to integrate this equation for G is

$$G(Z=0) = \frac{A_1}{F(0)} \frac{E(0)}{K(0)} \tag{21}$$

with the following expression for $F(0)$:

$$F(0) = \frac{\beta}{\left[1 + \frac{3}{2} C_{\varepsilon c} N_B/(\tau K^{1/2})(0)\right]} - \frac{1}{(c_m - 1/2)} \tag{22}$$

Asymptotic analysis : numerical results and comparison with experimental data

The evolution of $D_T(\widetilde{c})$ through the flame brush is shown in Fig. 2. In this figure we have represented the numerical results obtained by using the four algebraic models exposed in the previous sections. As stated above, $D_T(\widetilde{c})$ is evaluated from Eq. (8) and the turbulent flow field is assumed to be known from experimental data. In this calculation the various parameters introduced by the models have been given the values corresponding to the Li et al. experimental data [1],[17], namely $\tau = 6$, $N_B = 9.8$, $D_a = 51$, $d/w_1 = 8.3\ 10^{-3}\ s$, $S_l = 0.37\ ms^{-1}$. We have also reported the results obtained by using the classical relaxation model, i.e. $E_c \sim \widetilde{c}(1-\widetilde{c})E/K$, a model *a priori* valid to represent the dissipation of a passive scalar. The value of the constant introduced by this model is taken to be the same as the one of A_1/β in the Borghi and coworkers algebraic model. Though a scattering of the numerical data on both

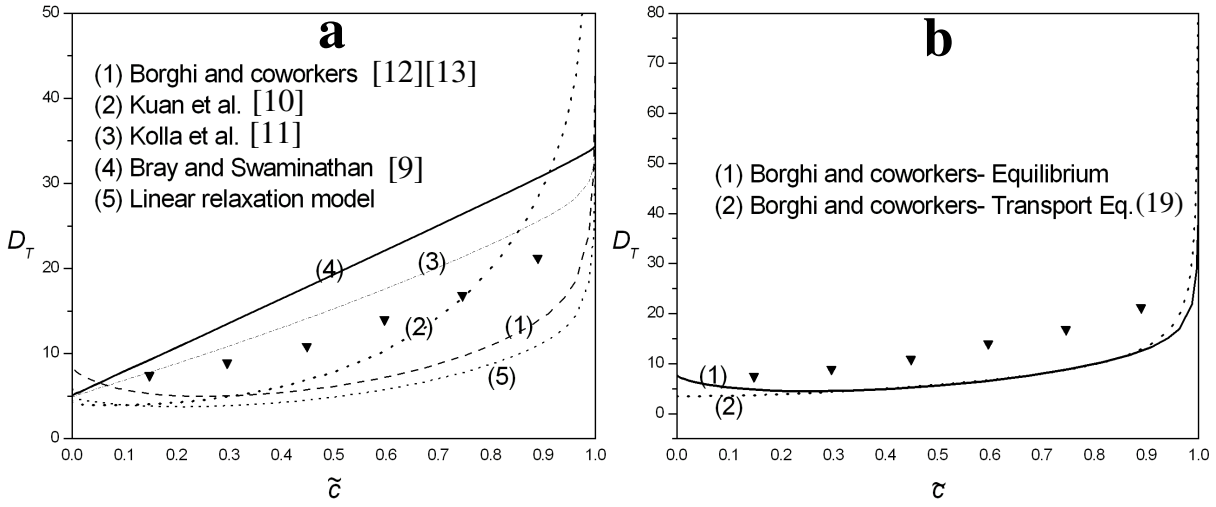

Figure 2: **a**: Comparison of models and deduced experimental distributions of D_T for the experimental data of Li et al. [1] (triangles), **b**: Comparison of calculations of D_T through the flame brush, using equilibrium and non equilibrium Borghi and coworkers models [12][13]

sides of the experimental points can be observed, it must be noted that qualitative evolution of D_T through the flame is correctly represented by the models. Both models of Bray and Swaminathan [9] and Kolla et al. [11] overpredict the evolution of D_T , though the agreement with the experimental data is much improved by the latter. It must be recalled here that the values of the various constants introduced by these two models have been given those obtained through comparisons with DNS data of planar turbulent flames (see [9] and [11]). An adjustment of these values would be needed to fair the numerical results with the experimental points. At the other end Kuan et al. and Borghi and coworkers models tend to underpredict the evolution of D_T and then of the mean chemical rate. Concerning the use of this model, Fig. 2-b provides a comparison between the evolution of D_T obtained from the algebraic model and the evolution of the same quantity obtained by solving the balance equation for the mean dissipation rate Eq. (19). The relatively small difference between the two calculations shows clearly that production terms on the RHS of Eq. (19) stay dominant through the flame brush, so that the equilibrium between these terms represented by the algebraic Borghi and coworkers model prevails. The mean structure of the turbulent flame within the stagnating flow is shown in Fig. 1-b.

This asymptotic analysis highlights two different model behaviours: (i) those directly connected to $\widetilde{\varepsilon}/\widetilde{k}$ i.e. the linear relaxation model, Kuan et al. model [10] and Borghi and coworkers model [12] [13] and (ii) those made of two contributions: one proportional to the inverse of the turbulent time scale $\widetilde{\varepsilon}/\widetilde{k}$ and another one proportional to the inverse of the laminar chemical time S_l/δ_l i.e. Bray and Swaminathan [9] and Kolla et al. [11]. It is found that the former tends to underpredict the evolution of D_T whereas the latter overpredicts the chemical reaction rate through the stagnating turbulent flames. Nevertheless, it must be also noticed that the models made of two contributions [9] [11] perform well as long as the values of the constants they involve are properly selected. To conclude, the experimental profile of D_T presented in Figure 2 can be well represented by using the models made of two contributions. On the contrary the profile obtained when using one of the models made of only one contribution does not fit the experimental data even by adjusting the model constants.

3D numerical simulations : description of the experimental test case and computational model

Results from a full three-dimensional numerical simulation of the stagnating turbulent premixed flame are now presented and discussed. The description of the experimental setup considered for the simulation can be found in the work of Cho et al. [2]. The corresponding turbulent reactive flow is sketched in Figure 1-a. The incoming flow impinges a wall located 7.5cm (d) downstream of the injection nozzle which has a diameter L of 5cm. The velocity w_1 at the exit of the nozzle is 5m/s and the incoming turbulence is generated by a grid. The equivalence ratio of the fully premixed methane-air mixture is unity and the jet is surrounded by a co-flow of air. The main characteristics of the flow are summarized in Table 1.

Table 1: Experimental conditions

Fuel	L	d	w_1	w_1'	l_T	Φ	τ	δ_L	S_L
CH_4	$5cm$	$7.5cm$	$5m/s$	$30cm/s$	$2mm$	1	6.7	$0,11mm$	$43cm/s$

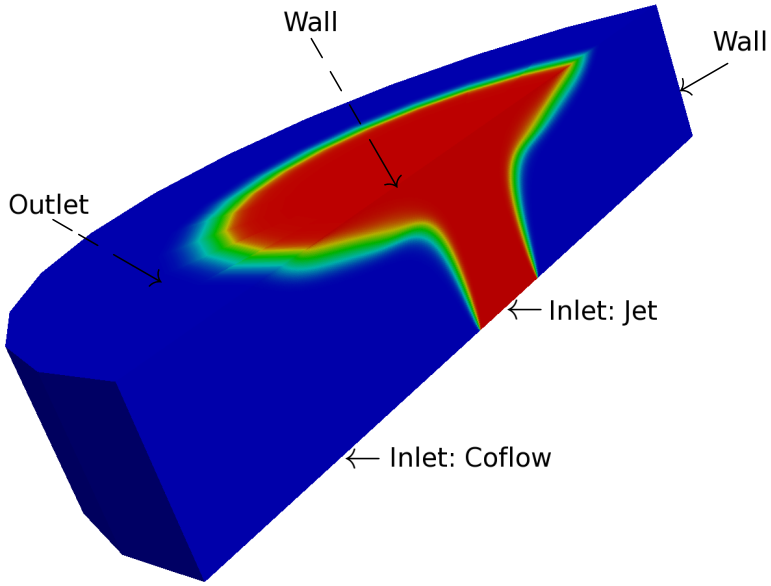

Figure 3: Mixture fraction on the boundaries of the three-dimensional computational domain

The computational domain has a diameter of $20cm$ and begins at the exit of the nozzle, it represents half of the physical space. The mesh is made up of 900000 cells. The impinging wall diameter is $10cm$. Figure 3 shows the mixture fraction field as obtained on the different boundaries of the three-dimensional computational domain.

Balance equations are solved for the momentum equation associated to a $\widetilde{k} - \varepsilon$ turbulence model and a mean progress variable transport equation, Eq.(2). The boundary conditions for turbulent quantity $\widetilde{k}$ and ε at the inlet jet of methane and air are respectively $\widetilde{k}_1 = 3/2w_1'^2$ and $\varepsilon_1 = c_\mu \widetilde{k}_1^{3/2}/l_T$ ($c_\mu = 0.09$). A passive scalar, i.e. mixture fraction, is also considered to follow the mixing between the coflow of air and the jet of reactants. It is important to notice that the key quantities for this turbulent reactive flow, namely mean progress variable and turbulence fields are now numerically caculated whereas in the above asymptotic analysis all these quantities were obtained from measurements.

The mean chemical source term is closed by using Eq.(3). Then, thanks to Eq.(3), two different algebraic models for the mean scalar dissipation rate, i.e. Bray and Swaminathan [9] described by Eq.(11) and Borghi and coworkers [12][13] described by Eq.(17), are evaluated on this geometry. These two models have been chosen as representative of the two different behaviours observed in the asymptotic analysis: (i) the Borghi and coworkers model is proportional to the inverse of a turbulent time scale whereas (ii) the Bray and Swaminathan model involves two terms, (i) one proportional to the inverse of a turbulent time scale and (ii) another one proportional to the inverse of a chemical time scale. It is noteworthy that, in this latter model, the term proportional to the turbulent time scale remains negligible everywhere. This characteristic is a consequence of the configuration considered characterized by a weak intensity of turbulence.

The turbulent scalar flux is represented by using either a gradient law (case GD) or an algebraic model able to deal with counter-gradient turbulent diffusion (case CGD). This latter

Table 2: Model constants retained in numerical simulations

	Gradient law (case GD)	Robin et al.[18] Eq.(23) (case CGD)
Bray and Swaminathan [9] Eq.(11)	$C_{\varepsilon c} = 0.10$, $\lambda = 0$ $C_{B1} = 0.07$, $C_{B2} = 0.21$	$C_{\varepsilon c} = 0.10$, $\lambda = 0.2$ $C_{B1} = 0.09$, $C_{B2} = 0.21$
Borghi and coworkers[12][13] Eq.(17)	$C_{\varepsilon c} = 0.10$, $\lambda = 0$ $A_1/\beta = 8$	$C_{\varepsilon c} = 0.10$, $\lambda = 0.2$ $A_1/\beta = 10$

model results from the recent proposal made by Robin et al.[18] and writes:

$$\overline{\rho u_k'' c''} = \left(\tau S_L \overline{\rho c''^2}\lambda - \overline{\rho}\nu_T/\sigma \|\nabla \widetilde{c}\|\right) \widetilde{M}_k \tag{23}$$

The flamelet assumption allows us to retain the maximum value of the scalar variance, i.e. $\overline{\rho c''^2} = \overline{\rho}\widetilde{c}(1-\widetilde{c})$. The parameter λ related to fluctuations of local flame normal vector [19] is considered to be constant in the simulation, (see Table 2). The turbulent viscosity is $\nu_T = c_\mu \widetilde{k}^2/\epsilon$. and the mean orientation of the turbulent scalar flux is approximated by the following relation: $\widetilde{M}_k = \nabla\widetilde{c}/\|\nabla\widetilde{c}\|$.

These models of turbulent combustion have been implemented in the Computational Fluid Dynamics (CFD) code developed by EDF: *Code_Saturne*, see Archambeau et al. [20]. *Code_Saturne* is a parallel general purpose three-dimensional low Mach number CFD code based on a finite volume method. The time marching scheme is based on a prediction of the velocity field followed by a pressure correction step. Equations for $\widetilde{k}$ and ε and scalars fields are resolved afterwards. Discretization in space is based on the fully conservative, unstructured finite volume framework, with a co-located arrangement for all variables.

3D numerical simulations : numerical results and comparison with experimental data

The model constants C_{B1}(Bray and Swaminathan model) and A_1/β (Borghi and coworkers model) used in the numerical simulations presented here, have been selected so that the obtained position of the calculated 3D turbulent flame is as realistic as possible. The BML constant c_m

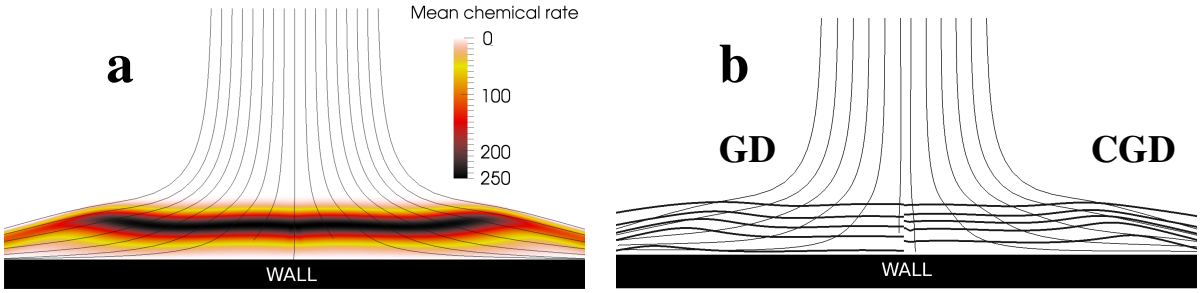

Figure 4: **a**: Numerical field of mean chemical rate $\overline{\omega}/\overline{\rho}$ (s^{-1}) and **b** Numerical streamlines and iso-c values (0.05, 0.25, 0.5, 0.75, 0.95) associated to a gradient law (left: case GD) and Robin and coworkers model [18] (right: case CGD) (Bray and Swaminathan model)

has been set to 0.88 in both cases. The numerical field of the mean chemical rate and the streamlines obtained by using the Bray and Swaminathan model are presented in Figure 4-a. Similar qualitative results are obtained by using either the Bray and Swaminathan model or the Borghi and coworkers model.

Figure 4-b shows streamlines and iso-values of the progress variable obtained by using either the gradient law or the Robin and coworkers model for the scalar turbulent flux [18]. As expected, taking into account the counter-gradient turbulent diffusion leads to a thinner and more realistic flame brush.

To conclude, it must be noticed that any of these models lead to a mean structure of the turbulent flame qualitatively similar to the one observed in experiments. Figure 5 shows the evolution of the progress variable and the axial velocity component along the symmetry axis. The two figures on the top have been obtained from a classical turbulent eddy viscosity assumption (GD approximation) whereas the two figures at the bottom have been obtained thanks to the generalized (case CDG) algebraic closure recently introduced by Robin et al. [18]. The profiles of the mean progress variable reported on the left side of Fig. 5 do not evidence strong differences between the results obtained by using (i) the model of Bray and Swaminathan, and (ii) the model of Borghi and coworkers. However the velocity profile is found to be much more sensitive to the choice retained for the representation of small scale scalar mixing effects. The corresponding results confirm that taking into account the chemical time scale δ_l/S_l

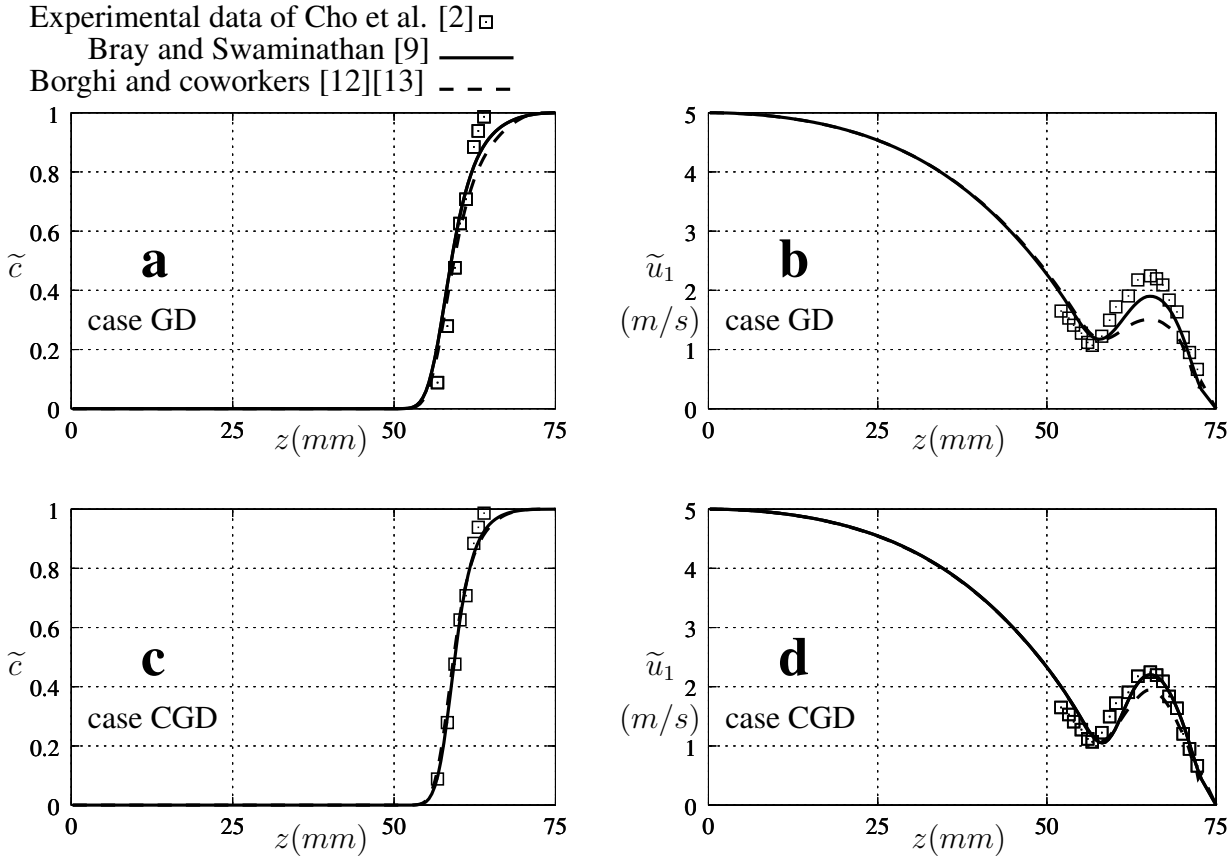

Figure 5: Comparison of the numerical profiles of the mean progress variable and axial velocity component along the symmetry axis with experimental data of Cho et al. [2], **a** and **b**: Gradient law, **c** and **d**: Robin et al. model for scalar turbulent flux [18]

improves the agreement between the results of numerical simulations and the available experimental data. Finally it is worth noting that the use of a turbulent transport closure that accounts for the possible occurence of counter-gradient diffusion effect also clearly improves the quality of the agreement obtained between experimental data and numerical simulations even for first moment quantities.

Conclusions

Various models for the mean scalar dissipation rate have been evaluated through their application to two different premixed turbulent flames stabilized in stagnating turbulence. In a first step these models are compared in the context of an asymptotic analysis conducted for small levels of incoming turbulence and large values of the Reynolds number. In this asymptotic analysis velocity field and scalar quantities are simultaneously used with models for the scalar dissipation rate. Models are then evaluated through a comparison with experimental data conducted in terms of a turbulent Damköhler number. In a second step of the investigation, a complete three-dimensional numerical simulation of the experimental setup is performed and the models for the scalar dissipation rate are evaluated in terms of the mean progress variable and the mean velocity field.

Two kinds of models can be identified, these directly connected to $\widetilde{\varepsilon}/\widetilde{k}$ i.e. the linear relaxation model, Kuan et al. model [10] and Borghi and coworkers model [12] [13] and those made of two contributions: one proportional to the inverse of the turbulent time scale $\widetilde{\varepsilon}/\widetilde{k}$ and another one proportional to the inverse of the laminar chemical time S_l/δ_l i.e. Bray and Swaminathan [9] and Kolla et al. [11]. It is found that the former kind tends to underestimate the chemical reaction rate whereas the latter overestimates the chemical reaction rate through the stagnating turbulent flame. Concerning now the transport equation for the mean scalar dissipation rate as applied to this situation of stagnating turbulent flames, results obtained by solving this transport equation are very closed to those obtained by considering the equilibrium of the dominant terms of this equation. This suggests that algebraic models for the mean scalar dissipation rate are appropriate to describe this kind of strained turbulent flames. Accordingly these algebraic closures have been retained to perform the three-dimensional numerical simulations of premixed flames in stagnating turbulence and it was found that the models made of two contributions [11] that include the influence of chemical time scale perform the best.

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