Small scale reactive scalar dynamics in turbulent premixed flames Part I: mean reactive scalar dissipation

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The present work is devoted to the analysis of reactive scalar dynamics in turbulent premixed flames from Direct Numerical Simulation (DNS) databases. The emphasize is on the behavior of small scale mixing terms of the reactive specie accross the flame brush. The starting point of the analysis is a transport equation for the mean scalar dissipation rate. The different terms of the corresponding budget are quantitatively evaluated from the DNS data. This is the first part of a more general study devoted to the characteristics of small scales in turbulent premixed flames. The second forthcoming part will focus on the conditional properties of these small scales.

1 Introduction

The relevance of scalar dissipation terms in the field of combustion is first briefly recalled. The most important idea to keep in mind is that molecular mixing is a prerequisite for combustion to occur. As a consequence, the scalar dissipation term that quantifies the local mixing rate is a key factor for combustion studies in almost all situations: i) molecular diffusion between burnt and unburnt gases for premixed reactants, ii) between fuel and oxidizer for diffusion flames or iii) combination of the two for non premixed or partially premixed situations. When turbulent combustion is considered, these molecular effects drive the evolution of the scalar statistics in the composition space through the scalar dissipation term together with chemical reaction. This can be evidenced by considering the Probability Density Function (PDF) formalism [1].

2 Mathematical concepts

Reactive scalar mixing description

From the instantaneous transport equation of a reactive scalar Y, the transport equation of the variance of this quantity is:

$$\begin{aligned}\frac{\partial\overline{\rho Y''^2}}{\partial t}+\frac{\partial\widetilde{u}_\alpha\overline{\rho Y''^2}}{\partial x_\alpha} &= \frac{\partial}{\partial x_\alpha}\left(\overline{\rho D\frac{\partial Y''^2}{\partial x_\alpha}}\right)+\overline{2Y''\frac{\partial}{\partial x_\alpha}\left(\rho D\frac{\partial\widetilde{Y}}{\partial x_\alpha}\right)}\\ &- \frac{\partial}{\partial x_\alpha}\left(\overline{\rho u''_\alpha Y''^2}\right)-2\overline{\rho u''_\alpha Y''}\frac{\partial\widetilde{Y}}{\partial x_\alpha}-\overline{2\rho D\frac{\partial Y''}{\partial x_\alpha}\frac{\partial Y''}{\partial x_\alpha}}+2\overline{\rho w_Y Y''}\end{aligned} \quad (1)$$

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The fifth term of the Right Hand Side (RHS) of Eq. (1) is the fluctuating part of the mean dissipation term $\widetilde{\epsilon_Y}$ on which attention is focused in the following sections.

Reactive scalar PDF evolution
The evolution equation for the PDF $\widetilde{P} = \widetilde{P}(Y^*)$ writes [1]:

$$\frac{\partial \widetilde{P}}{\partial t} = -\frac{\partial}{\partial Y^*}\left(\left\langle \frac{\partial Y}{\partial t}|Y^*\right\rangle \widetilde{P}\right) = -\frac{\partial}{\partial Y^*}\left(\left\langle \frac{\partial u_\alpha Y}{\partial x_\alpha} + \frac{1}{\rho}\frac{\partial}{\partial x_\alpha}\left(\rho D \frac{\partial Y}{\partial x_\alpha}\right)|Y^*\right\rangle \widetilde{P} + w_Y(Y^*)\widetilde{P}\right) \quad (2)$$

where the second term of the RHS can be rewritten as follows to evidence the role of the conditional scalar dissipation $\langle \epsilon_Y | Y^* \rangle$:

$$\frac{\partial}{\partial Y^*}\left(\left\langle \frac{1}{\rho}\frac{\partial}{\partial x_\alpha}\left(\rho D \frac{\partial Y}{\partial x_\alpha}\right)|Y^*\right\rangle \widetilde{P}\right) = \frac{1}{\overline{\rho}}\frac{\partial}{\partial x_\alpha}\left(\overline{\rho D}\frac{\partial \widetilde{P}}{\partial x_\alpha}\right) + \frac{1}{\overline{\rho}}\frac{\partial^2}{\partial Y^* \partial Y^*}\left(\left\langle \rho D \frac{\partial Y}{\partial x_\alpha}\frac{\partial Y}{\partial x_\alpha}|Y^*\right\rangle \widetilde{P}\right)$$

Flame surface density function
Transport equations can be also derived for the flame surface density function $\Sigma(Y^*) = \langle \|\nabla Y\| | Y^* \rangle \widetilde{P}$. Since strong relationships exist between instantaneous scalar gradients and scalar dissipation, some similarities with the previous formalisms can be evidenced as discussed for instance by Pope [2].

Finally, these mathematical preliminaries clearly evidence that, whatever the point of view adopted to deal with turbulent combustion modelling, scalar dissipation is a key quantity.

	case H	case M	case L
ρ_u/ρ_b	7.530	5.000	2.500
S_L (m/s)	0.600	0.523	0.416
δ_L (mm)	0.217	0.191	0.158
u'/S_L	0.880	1.010	1.260

Table 1: Characteristics of the Direct Numerical Simulation databases

3 Diagnostics from the DNS databases

Fully developed turbulent premixed flames have been obtained for three different values of the density ratio and using a single-step irreversible reaction, while the turbulent intensity was comparable to the laminar burning velocity. The Reynolds number based on the integral scale is Re_{lt}=95.5 for the three databases and the resolution is 512*128*128. The numerical methodology relies on a spectral collocation method for direction y and z, whereas a sixth order finite differences scheme with spectral like resolution has been used along direction x. Third order Runge Kutta scheme is used for time integration. Other details concerning the simulations have been provided elsewhere [3], and the conditions are summarized in Tab. 1. In the present simulation databases [3], the flame propagates along the x-direction and ensemble averaging is performed in the (y,z) planes. Moreover, since the flame is stationnary in the mean sense [3], the procedure is not only performed by slicing the DNS database in planes normal to the direction of the mean planar flame propagation but also by averaging the results in time by using an appropriate sampling period. Constant progress variable iso-surface c=c_f may be used conveniently to define the flame front location. Here, the flame surface density $\Sigma(c_f)$ is obtained following the procedure proposed by Trouvé and Poinsot [4]. The influence of the choice of c_f has been investigated and is illustrated in Fig. 1 for the case H that corresponds to the highest density ratio accross the flame brush. Results are made non dimensional by using the acoustic velocity in the unburnt gases (c_0= 387 m/s) and the length of the computational domain (L= 4 mm).

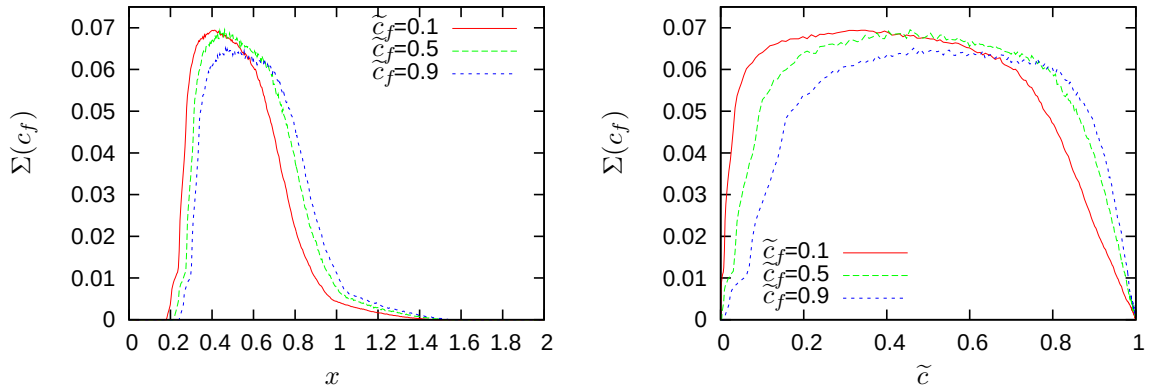

Figure 1: Case H: the mean flame surface density $\Sigma(c_f)$ as a function of the distance x accross the flame brush (left) and of the mean progress variable (right).

4 Mean reactive scalar dissipation

The first step of the present analysis is to consider the unclosed equation for the mean dissipation of the reactive scalar Y. Such an equation has been discussed for instance in [5, 6] and taking the density variations into account, the transport equation writes:

$$\begin{aligned}\frac{\partial \overline{\rho\epsilon_Y}}{\partial t} &= \underbrace{-\frac{\partial}{\partial x_i}\left(\widetilde{U_i}\overline{\rho\epsilon_Y}\right)}_{\text{(II)}} + \underbrace{\frac{\partial}{\partial x_i}\left(\overline{\rho\, D\frac{\partial \epsilon_Y}{\partial x_i}}\right)}_{\text{(III)}} \underbrace{-\frac{\partial \overline{\rho u_k'' \epsilon_Y}}{\partial x_k}}_{\text{(IV)}} \underbrace{-2\overline{\rho D\frac{\partial Y''}{\partial x_i}\frac{\partial u_k''}{\partial x_i}\frac{\partial \widetilde{Y}}{\partial x_k}}}_{\text{(V)}} \underbrace{2\overline{\rho D\frac{\partial Y''}{\partial x_k}\frac{\partial Y''}{\partial x_i}\frac{\partial \widetilde{U_k}}{\partial x_i}}}_{\text{(VI)}} \\ &- \underbrace{2\overline{\rho D u_k''\frac{\partial Y''}{\partial x_i}\frac{\partial^2 \widetilde{Y}}{\partial x_k \partial x_i}}}_{\text{(VI-b)}} \underbrace{-2\overline{\rho D\frac{\partial Y''}{\partial x_k}\frac{\partial Y''}{\partial x_i}\frac{\partial u_k''}{\partial x_i}}}_{\text{(VII)}} \underbrace{-2\overline{\rho D^2\frac{\partial^2 Y''}{\partial x_k \partial x_i}\frac{\partial^2 Y''}{\partial x_k \partial x_i}}}_{\text{(VIII)}} \underbrace{-2\overline{\rho D\frac{\partial Y''}{\partial x_i}\frac{\partial \omega_Y}{\partial x_i}}}_{\text{(IX)}} \\ &+ \underbrace{2\,\overline{\rho D\frac{\partial Y''}{\partial x_i}\frac{\partial}{\partial x_i}\left(\frac{1}{\rho}\right)\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial Y}{\partial x_j}\right)}}_{\text{(X)}} + \underbrace{2\,\overline{D\frac{\partial Y''}{\partial x_i}\frac{\partial}{\partial x_j}\left(D\frac{\partial Y}{\partial x_j}\frac{\partial \rho}{\partial x_i}\right)}}_{\text{(XI)}} \end{aligned} \quad (3)$$

In the previous equation, constant diffusivity has been assumed but others forms (not reported here) that do not rely on this hypothesis have also been derived. The different terms are displayed in Fig.(2). Their respective orders of magnitude are consistent with the analysis given in previous works [5, 6] but it must be noticed that the contribution of turbulent straining term (VII) appears as a sink term whereas it has been considered as a production term balancing term (VIII) in earlier works. The dominant terms are the dissipation term (VIII) and the chemical term (IX). At a lower order we find that the turbulent straining term and one of the term related to density-variations i.e. term (X) play also a significant role. The influence of this last contribution was not taken into account in almost all previous works.

5 Conclusions

The present work gives new insights concerning the balance of dominant terms in the mean disipation equation. In particular, at leading order, the balance between (VIII) and (IX) is recovered as expected

when considering laminar flamelets. Concerning the closure of the correlations present in the RHS of Eq. (2), additional investigations based on a previous modelling proposal [5] show a very good agreement with the DNS data for certain terms but others still require further improvements. At lower order, it is found that one among the different term, related to variable density effects, is balanced by the velocity to scalar fluctuations correlation, namely the term (VII). This latter term appears as a sink term for the mean dissipation, a feature in contradiction with all previous modelling proposals. The amplitudes of terms (VII) and (X) are found to decrease as the density ratio between fresh and burned gases is decreased but (VII) remains always negative. This complex and interesting behavior is quite different from the one observed for passive scalars in turbulent flows.

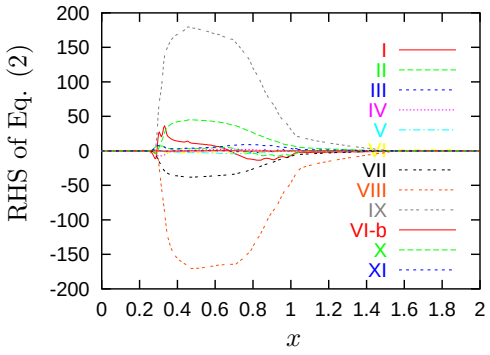

Figure 2: Case H: streamwise balance of production rates of reactive scalar dissipation given by Eq. (3).

From the modelling point of view, the term (VII) is expected to depend on the density ratio and the use of the three present DNS databases will be helpful in this purpose. The term (X) plays also a significant role, the orders of magnitude of the scalar and density gradients are not too difficult to find but this term also requires the knowledge of second order derivatives of Y. Consideration of the balance within a one-dimensional laminar premixed flame will help us to estimate this last contribution.

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