Modelling of premixed turbulent combustion with variable equivalence ratio using a new « partial pdfs » approach

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1. Abstract

The present study is a new step towards the modelling of complex situations such as turbulent combustion with premixed but non necessarily well homogeneous reactants, herein an original approach to tackle the problem of prediction of the pdf of reactive species is proposed. Practically, turbulent combustion calculations are performed by numerical integration of modelled equations. In usual approach of turbulence, the whole contribution of fluctuations is modelled, whereas in Large Eddy Simulation methods, only effects of fluctuations occuring at scales smaller than resolved have to be estimated. Generally, chemistry is relatively fast so that combustion takes place at scales smaller than resolved, thus the modelling problem of interaction between turbulence and reaction remains. In the paper, a new approach called Partial Pdf Method is proposed and tested ; it can be viewed as an extension of classical and widely used method of presumed pdf and allows to deal with more complicated forms of pdf than previously done and without having the numerical costs of calculated pdf approach. It is used within the conventional moment approach of turbulence but can also be of interest for LES methodology. In this new method, equations describing the evolution of portions of the pdf are deduced from the modelled balance equation of the whole pdf. Then, balance equations for the weight of each portion, its position and thickness in the sample space are derived and the entire pdf is simply recontructed by a weighted average of partial pdfs. Finally, the method is used to simulate an highly stretched turbulent premixed flame.

2. Introduction

There are many problem of practical interest where a flame propagates into a non homogeneous premixed medium, direct fuel injection engine is one of the most common example. In that case, the problem is not simply related to the estimation of the flame surface density or the reactive scalar dissipation rate. Indeed, fluctuations of mixture fraction must be accounted for so that a joint pdf of mixture fraction and reactive species is necessary. In fact, to represent the thermodynamical state of a non homogeneous burning mixture, under the assumption of equal diffusivities and of a single reaction (or at least supposing that the whole kinetic description can be represented with a single progress variable), we need only three variables, the first one represents the mixing of reactants at the largest scales ; it is called mixture fraction Z, the second one is used to characterise the reaction progress ; we choose here the oxidiser mass fraction Y_{O_2}, the last one is the total enthalpy of the system H. To evaluate the mean reaction rate, knowledge of the joint probability density function $P(Y_{O_2}, Z, H)$ is necessary. In the case of very fast reaction, this pdf is bimodal in the Y_{O_2} direction, but this may not be realistic for suffiently fuel lean mixtures. If it is supposed that H is only related to Z and T_0 with T_0 the temperature in the fresh mixture, then the knowledge of $P(Y_{O_2}, Z)$ is sufficient.
So, to account for fluctuations of mixture fraction, the joint pdf of mixture fraction and reactive specie is necessary. Some authors recently tried to extend flamelet models to premixed combustion with variable equivalence ratio for example with BML type model (Lahjaily *et al.* (1998), *ref.* [7]) or with flame surface density type models (Hélie & Trouvé (2000), *ref.* [6]). In fact, it seems to be relatively difficult to extend those models to the case with non homogeneous reactants, because not only the mean equivalence ratio varies from place to place but it does also fluctuate as well as velocity or temperature. The problem is to evaluate the mean reaction rate which is distributed along the surface of flamelet but in this case the equivalence ratio of a portion of flamelet can differ from the neighbouring portion. This induces different speeds of propagation for each portion of flamelet and the propagation speed of a given portion will depend on the local equivalence ratio but also on that of its neighbours. This will induce an

additionnal stretch specifically due to partial premixing (Poinsot *et al.* (1996), *ref.* [10]). In principle, the problem can be attacked using a full pdf calculation, but it remains relatively time consuming. Moreover, multi-dimensionnal presumed pdf using multivariate beta distribution (Girimaji (1991), *ref.* [5]) remains questionnable if reactive scalar is involved. Usually, the problem is eluded by using an hypothesis of statistical independance between stochastic variables. It is also often assumed that fluctuations of mixture fraction only occurs in burnt and unburnt gases. These assumptions are not really justified. Here, an approach allowing to take into account arbitrary two or three dimensionnal pdf is proposed.

3. Partial Pdf - Scalar Dissipation Modelling

In the case of very fast chemistry with homogeneous reactants, a one dimensionnal bimodal pdf is expected and it is well known that mean reaction rate is directly proportionnal to the mean scalar dissipation of the fluctuations of reactive specie or to the flame surface density (Borghi (1990), *ref.* [2]). In fact, if chemistry is sufficiently fast, solving a modelled equation for mean scalar dissipation allows to get the mean reaction rate in the form of a modified EBU type model (Mantel & Borghi (1994), *ref.* [8] and Mantel *et al.* (1997), *ref.* [9]). Flamelet structures were first incorpated in fast chemistry or mixing controlled model of turbulent combustion via algrebraic relations (Said & Borghi (1988), *ref.* [1]) and play a very important role in the modelling of the scalar dissipation equation. The Mantel & Borghi equation for scalar dissipation was strictly derived for very fast chemistry but its range of application probably exceeds this restricted regime: the presence of flamelet structures, even partially perturbed by turbulence is enough to justify the closure. Moreover, it is possible to extend this equation to the case of non constant equivalence ratio taking additional stretch due to stratification into account.
However, we are interested in the general case where the mean reaction rate is not directly proportionnal to $\widetilde{\epsilon_{Y_{O_2}}}$, then the joint pdf transport equation $P(Y_{O_2}, Z)$ jointly with an equation for $\widetilde{\epsilon_{Y_{O_2}}}$ can be used. It can account for flamelet occurence and extinction with a suitable micro mixing model. In *ref.* [4], a transport equation for the joint pdf $P(Y_{O_2}, Z)$ has been written and a closure supplied for micro mixing term. The flamelet structure has been taken into account following the approach of Pope & Anand (1984) (*ref.* [11]). It is important to emphasize that the micro mixing time scale has to be calculated through $\widetilde{\epsilon_{Y_{O_2}}}$ equation and not taken directly proportionnal to k/ϵ.

The calculation of this pdf with usual Monte Carlo simulation is quite time consuming. Here, we propose a new method in order to built approximated forms of this two dimensionnal pdf. Fisrt, we decomposed it in the following way:

$$P(Y_{O_2}, Z, \boldsymbol{x}, t) = P(\boldsymbol{C}, \boldsymbol{x}, t) = \sum_{i=1}^{i=n} \alpha_i(\boldsymbol{x}, t)\, \phi^i(\boldsymbol{C}, \boldsymbol{x}, t) \quad \text{with} \quad \boldsymbol{C} = \begin{pmatrix} Y_{O_2}(\boldsymbol{x}, t) \\ Z(\boldsymbol{x}, t) \end{pmatrix} \tag{1}$$

Each $\phi^i(\boldsymbol{C}, \boldsymbol{x}, t)$ is a partial pdf (that point will be examined in further details in the application) and α_i is the relative weight of that partial pdf. Once partial pdfs are reconstructed the whole pdf is simply obtained by a weighted average of partial pdfs.

The following normalization conditions must be checked :

$$\sum_{i=1}^{i=n} \alpha_i(\boldsymbol{x}, t) = 1 \quad \text{and} \quad \int_{\boldsymbol{C}^*} \phi^i(\boldsymbol{C}^*, \boldsymbol{x}, t) d\boldsymbol{C}^* = 1 \tag{2}$$

Inserting (1) in the modelled pdf equation and integrating, it is found that the weighting coefficient $\alpha_i(\boldsymbol{x}, t)$ follows a simple turbulent advection diffusion equation.

$$\frac{\partial \overline{\rho} \alpha_i}{\partial t} + \frac{\partial}{\partial x_k} \left(\overline{\rho} \widetilde{u_k} \alpha_i \right) = \frac{\partial}{\partial x_k} \left(\overline{\rho} D_t \frac{\partial \alpha_i}{\partial x_k} \right)$$

One can also derive an equation for $\phi^i(Y_{O_2}, \boldsymbol{x}, t)$:

$$\frac{\partial \overline{\rho} \phi^i}{\partial t} + \frac{\partial}{\partial x_k} \left(\overline{\rho} \widetilde{u_k} \phi^i \right) = \frac{\partial}{\partial x_k} \left(\overline{\rho} D_t \frac{\partial \phi^i}{\partial x_k} \right) - \frac{\partial}{\partial Y^*_{O_2}} \left(\overline{\rho} \left(\frac{Y^*_{O_2} - \widetilde{Y_{O_2}}}{\tau_{Y_{O_2}}} + \omega_{Y^*_{O_2}} \right) \phi^i \right) + 2 \frac{\overline{\rho} D_t}{\alpha_i} \frac{\partial \alpha_i}{\partial x_k} \frac{\partial \phi^i}{\partial x_k}$$

For the first order moment, we get :

$$\frac{\partial \overline{\rho}(\widetilde{Y_{O_2}})_i}{\partial t} + \frac{\partial}{\partial x_k}\left(\overline{\rho}\widetilde{u_k}(\widetilde{Y_{O_2}})_i\right) = \frac{\partial}{\partial x_k}\left(\overline{\rho}D_t\frac{\partial(\widetilde{Y_{O_2}})_i}{\partial x_k}\right) - \overline{\rho}\frac{(\widetilde{Y_{O_2}})_i - \widetilde{Y_{O_2}}}{\tau_{Y_{O_2}}} + \overline{\rho}(\widetilde{\omega_{Y_{O_2}}})_i + 2\frac{\overline{\rho}D_t}{\alpha_i}\frac{\partial \alpha_i}{\partial x_k}\frac{\partial(\widetilde{Y_{O_2}})_i}{\partial x_k} \tag{3}$$

For the second moment :

$$\frac{\partial \overline{\rho}(\widetilde{Y^2_{O_2}})_i}{\partial t} + \frac{\partial}{\partial x_k}\left(\overline{\rho}\widetilde{u_k}(\widetilde{Y^2_{O_2}})_i\right) = \frac{\partial}{\partial x_k}\left(\overline{\rho}D_t\frac{\partial(\widetilde{Y^2_{O_2}})_i}{\partial x_k}\right)$$

$$- 2\overline{\rho}\frac{(\widetilde{Y^2_{O_2}})_i - (\widetilde{Y_{O_2}})_i\widetilde{Y_{O_2}}}{\tau_{Y_{O_2}}} + 2\overline{\rho}(\widetilde{\omega Y_{O_2}})_i + 2\frac{\overline{\rho}D_t}{\alpha_i}\frac{\partial \alpha_i}{\partial x_k}\frac{\partial(\widetilde{Y^2_{O_2}})_i}{\partial x_k} \tag{4}$$

For partial mixture fraction moments, equations are similar but without chemical source terms and with $\tau_Z = \widetilde{Z''^2}/\widetilde{\epsilon_Z}$ instead of $\tau_{Y_{O_2}} = \widetilde{Y''^2_{O_2}}/\widetilde{\epsilon_{Y_{O_2}}}$. Concerning the chemical source term, we use a simple Arrhénius law (Westbrook & Dryer (1984), *ref.* [13]), it is necessary to now approximate forms for partial pdf in order to compute it.

Using partial pdfs, which only represent a portion of the total pdf in the sample space, the usual approximation of statistical independance of stochastic variables is a better approximation than when considering the whole pdf. In the following application, we will use that approximation which allows to deal with the joint partial pdf as the product of unidimensionnal partial pdfs.

So, we have : $\phi^i(\boldsymbol{C}, \boldsymbol{x}, t) = \phi^i(Y_{O_2}, \boldsymbol{x}, t)\ \phi^i(Z, \boldsymbol{x}, t)$ (5)

Partial pdfs can be approximated by presumed forms with three parameters such as beta functions or Dirac peaks and rectangles (Borghi (1988), *ref.* [1]). Here we assumed beta distribution for mixture fraction partial pdfs and Dirac peaks and rectangles for reactive scalar partial pdfs. At this point, it is important to note that with this approach complex forms of pdf can be reconstructed. Those complex forms are often found in experiments, for example when investigating a flame anchored by means of a pilot flame, multi modal pdf forms are observed and it can not be represented by simple bimodal form of beta type but partial pdfs method have the potential to deal with that type of pdf. Within this presumed partial pdfs framework, only the first two partial moments are necessary.

This method appears as an intermediate approach between the full presumed pdf methods where the pdf is reconstructed from its first and second moments and the Monte Carlo simulation where the pdf is built with a sum of partial pdf with the shape of a Dirac peak. The number of partial pdfs here is at choice of the user. The quality of the result depends on this number and on the shape of the partial pdf choosen.

4. Application to Highly Stretched Turbulent Premixed Flame

As a test case, we choose the experimental configuration of highly stretched flames of RWTH Aachen. It consists in a piloted Bunsen burner with a nozzle diameter of 12 mm issuing in air environment at three different mean nozzle exit velocity (65 m/s [F1 flame], 50 m/s [F2 flame] and 30 m/s [F3 flame]). We essentially concentrate our attention on the F2 and F3 flames of this well documented experiment. A schematic diagram of the Bunsen burner with enlarged pilot flame is depicted on Figure 1.

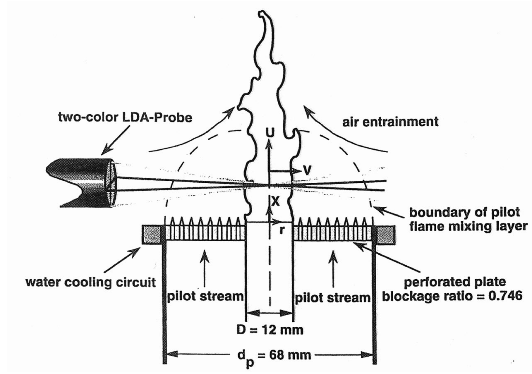

FIG. 1: *Experimental configuration of Chen et al., ref. [3]*

In this application, we considered that angle between mean normal direction to flamelet and mean direction of variation of mixture fraction is sufficiently low to neglect the additional stretch term in the $\widetilde{\epsilon_{Y_{O_2}}}$ equation. We use only three partial pdfs for the calculation, the first one is related to fresh mixture coming from high speed jet, the second to the coflow of burned mixture and the last corresponds to ambiant air.

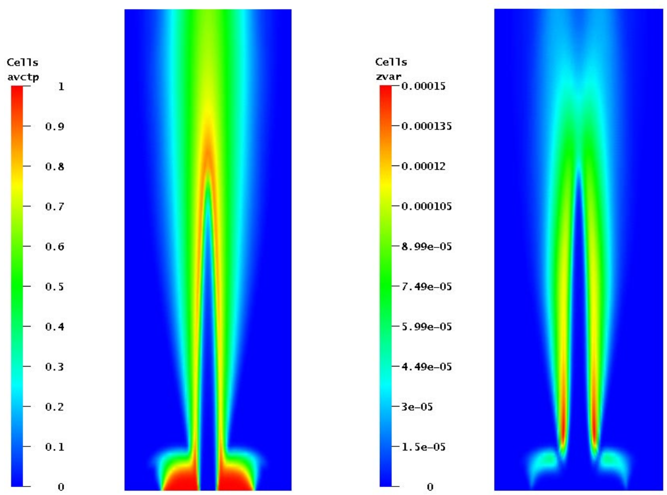

FIG. 2: *Mean progress variable contours* $c_T(\boldsymbol{x},t) = (\widetilde{T}(\boldsymbol{x},t) - T_u)/(T_{ad}(Z_{st},T_u) - T_u)$ *with* $T_u = 298$ *K & mixture fraction fluctuations for F3 flame*

On Figure 2 (left hand side), the mean reduced temperature (or progress variable based on temperature) is shown for flame F3. The distribution clearly displays the contribution of turbulent convection on the flame structure. The flame temperature progressively increases in the down-stream direction up to the values close to the adiabatic temperature (red on the figure). Mixture fraction fluctuations can be seen on the same figure (right hand side) here the mixture fraction is defined following diffusion flame formalism, so that its value is null in the air and unity in pure fuel (for beta pdf calculations, we used $Z_N(\boldsymbol{x},t) = Z(\boldsymbol{x},t)/Z_{st}$). On the Figure 3, profiles for mean progress variables and vertical component of velocity are represented in the case of flame F3. They are in qualitative agreement with experimental results from *ref.* [3]. The aims are to get a realistic description of flame structure and to compare results of partial pdfs calculations to that obtained with a full presumed pdf method or calculated pdf with lagrangian Monte Carlo approach.

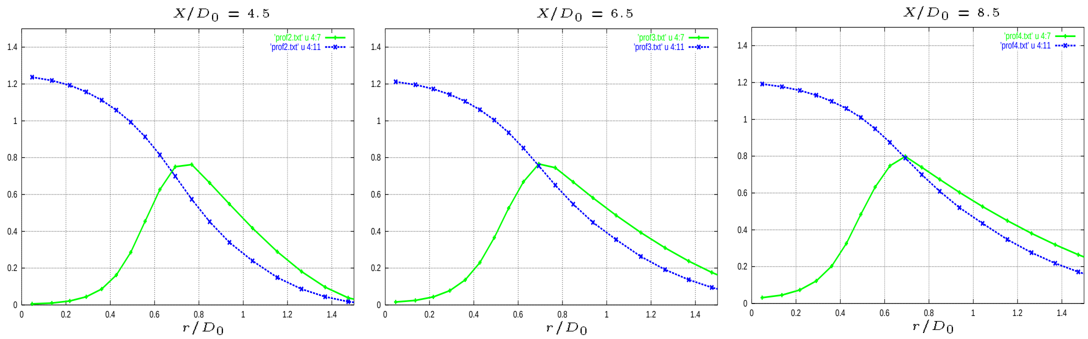

FIG. 3: *Mean progress variable & mean velocity profiles for F3 flame*

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