Modelling of Premixed Turbulent Combustion for Smart Control

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I. Introduction

Smart control is now increasingly considered in the design of combustion chambers, in order to suppress combustion instabilities or, at the contrary, to organize pulsating regimes. It is of interest for the design and operation of such devices to take advantage of prediction models for turbulent combustion, and the ability of such models of representing unsteady processes is of new and primary importance.
Even in the case of small devices, Direct Numerical Simulation is too expensive, and it is necessary to model the effects of the thin flamelets and reactive structures that are imbedded in the flame brush. Due to the interest in unsteady regimes, the Large Eddy Simulation (LES) approach is in order. Indeed, the objective of modelling unsteady combustion is not new, and the oldest numerical models that were built for reciprocating engines (like the code "Conchas") in the sixties were using the LES approach. But the proper characteristics that are needed for correctly representing unsteady large scale phenomena were not really known at this time. We have learn a lot since this period concerning the turbulent fluxes in combusting media, concerning the turbulence modification due to combustion, and concerning the influence of flamelets on the subgrid scale reaction rate. All this knowledge has been mainly used for Reynolds Averaged Navier Stokes (RANS) models, but has also to be used for the building of LES subgrid scale models. It is then of interest to see whether or not the existing LES models for turbulent combustion are in agreement with this knowledge.
The purpose of this paper is to present a synthetic picture of the interesting features of Turbulent Combustion Modelling methods of LES type, with some discussions of the strong and weak points of the available models. As a basic example of the premixed burner that is of interest for us, we can consider the schematic drawing of Fig. 1. The turbulent flame is stabilized more or less firmly by a flame holder, and is basically oblique with respect to the main flow. But in some circumstances, flash-back events may occur in which the flame brush can go upstream the flame holder and can lie perpendicularly to the main flow.

II. Turbulent combustion models for infinitely fast chemistry

We consider first the case of very fast chemistry because this case is of clear practical interest, but also simply as a first step in the discussion of the full problem. In this case, and for sufficiently large Reynolds number, the flame brush is composed of wrinkled flamelets ; when the chemistry is infinitely fast, the flamelets cannot be extinguished by the stretching and do keep a structure very close to the one of laminar steady flamelets. It is clear in this case that, even if the LES approach uses a grid whose size is smaller than the one of a RANS approach, the grid size will remain much larger than the flamelet thickness, and consequently the subgrid scale reaction rate cannot be represented by an Arrhenius-like formula. The problem is exactly the same as for RANS models in this very fast chemistry case.

II.1 Existing models and their weak points

The first, oldest, model considers that the very thin flamelets can be artificially thickened in such a way their structure can be solved satisfactorily with the coarse grid. This

is done using the subgrid scale eddy diffusivity instead of the molecular one, and keeping an Arrhenius law for the subgrid scale reaction rate. Then, the balance equation for the "mean subgrid scale progress variable" is the same as the usual one :

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{c})+\frac{\partial}{\partial x_\alpha}(\overline{\rho}\widetilde{c}\widetilde{v}_\alpha)=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial\widetilde{c}}{\partial x_\alpha}\right)+K_{SG}Y(\widetilde{c})Y_O(\widetilde{c})\exp(-\frac{T_A}{\widetilde{T}(\widetilde{c})}) \quad (1)$$

In this formula, of course, the Reynolds and Favre mean values are obtained with a certain spatial and temporal filter, which smooth only the subgrid scale fluctuations. D_{SG} is the subgrid scale eddy diffusivity, and K_{SG} the preexponential factor. As proposed in the seventies by Butler and O' Rourke, this factor has to be modified with respect to its value for laminar flames. But the question of how much the preexponential factor has to be diminuished is difficult (see Colin et al. [1]). It is clear that this formula do represent the "subgrid scale mean flamelet" and the numerical value of this factor is directly related to the mean velocity of propagation of this mean flamelet. This velocity depends on the turbulence length scale and velocity scale, at the subgrid scale only, but this dependence is not well known. In addition, the reaction rate of the subgrid scale mean flamelet does not depend on the mean subgrid scale progress variable as asymmetrically as in the Arrhenius law, because chemistry is not the only phenomenon implied. Then, such an Arrhenius shape is not at all justified.

Of course, another problem is posed by the subgrid scale eddy diffusivity. Up to now, classical models used for non reactive flows are used, as the Smagorinsky or the Germano model. The same approach is used in all the other models used so far, and this problem will be discussed in the section II.3.

The second model comes directly from the consideration that the problem of mean reaction rate is the same for LES approach and for RANS approach. Then, for a wrinkled flame, the popular BML model can be applied, which is very close to the so called "Eddy Break Up" model (see K.N.C.Bray [2], or [3]). Then the equation for the subgrid mean progress variable becomes :

$$\frac{\partial}{\partial t}(\overline{\rho}\widetilde{c})+\frac{\partial}{\partial x_\alpha}(\overline{\rho}\widetilde{c}\widetilde{v}_\alpha)=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial\widetilde{c}}{\partial x_\alpha}\right)+C_{SG}\frac{\widetilde{c}(1-\widetilde{c})}{T^t_{SG}} \quad (2)$$

There is a time scale at the denominator of the mean reaction rate, that is intended to be related only to the subgrid scale turbulence, and not to chemistry, as shown in the BML theory. Under its simplest form, i.e. with the factor C_{SG} constant, this model has been used by Fureby et al., with realistic results [4]. The dependence on the mean progress variable here is much more realistic than in the previous model, and in agreement with the BLM theory (which predicts also a weaker dependence of C_{SG} on this progress variable, due to density variations).

A third model, which is physically based on the picture of a "mean subgrid scale flamelet" that propagates with a "mean flamelet velocity", can be derived from the so-called G-equation that has been used for DNS in turbulent combustion. When considering a very thin flamelet whose laminar velocity of propagation is well known (not necessarily constant), the instantaneous position of the flamelet can be followed with the equation for G($\underline{x}$,t):

$$\rho\frac{\partial}{\partial t}(G)+\rho V_\alpha\frac{\partial}{\partial x_\alpha}(G)=\rho_u S_L|\nabla G|$$

The flamelet position is at a given, constant, value of G, G being a continuous function of x and t, contrary to the progress variable c itself that takes only the values zero or one. For the LES model, we cannot follow the instantaneous G, but we want to follow its subgrid scale mean value, and a very simple model for that is to assume the balance equation :

$$\overline{\rho}\frac{\partial}{\partial t}(\widetilde{G})+\overline{\rho}\widetilde{v}_\alpha\frac{\partial}{\partial x_\alpha}(\widetilde{G})=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial\widetilde{G}}{\partial x_\alpha}\right)+\rho_u S_T|\nabla\widetilde{G}|$$

Then, the mean value of G can be identified with the mean value of the progress variable, when the boundary and initial conditions are chosen the same, and we get, using the mean continuity equation, a new model :

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{c}\right)+\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}\widetilde{c}\widetilde{v}_\alpha\right)=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial\widetilde{c}}{\partial x_\alpha}\right)+\rho_u S_T\left|\nabla\widetilde{c}\right| \qquad (3)$$

Such a model has been used by Menon et al. [5], and Boger et al.[6]. The same model has been independently proposed in the framework of RANS by Weller et al. [7] and by Zimont et al. [8]. In the framework of LES, S_T is the velocity of propagation of the mean subgrid scale flamelet, while it is the classical turbulent flame speed in the RANS framework. In both cases, this quantity is not well known, and this is a shortcoming of this model. On the other hand, it can be seen that this model has a strongly non realistic behavior in the simple case of a one dimensional flame propagating in a constant turbulent field. Indeed, if we rewrite in this case the mean progress variable equation, we find a simple convection-diffusion equation, without any reaction term :

$$\overline{\rho}\frac{\partial}{\partial t}\left(\widetilde{c}\right)+\overline{\rho}\left(\widetilde{v}-\frac{\rho_u}{\overline{\rho}}S_T\right)\frac{\partial}{\partial x}\left(\widetilde{c}\right)=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial\widetilde{c}}{\partial x_\alpha}\right)$$

The solution of this equation, the initial condition being any realistic mean progress profile, is a continuous displacement and continuous thickening of this profile. Then, this model finds that there is no steady mean flame brush along the propagation ! Of course, it is very difficult to experimentally assess that a turbulent flame propagating in constant turbulence will reach a steady propagation (in the sense of mean values, of course), but this property was commonly conjectured and a recent DNS do show this property without any doubt, see Nishiki et al. [9]. The figures 2 and 3 do show that.

Nevertheless, this model gives very realistic results when applied only for finite times or in relatively short combustors. The problem of the lack of predictability due to the bad knowledge of S_T , as a function of subgrid scale turbulence, is more important…

II.2 Introducing an improved model

The application of the BML model for LES in case of very fast reactions seems then the best base for deriving a satisfactory model. However, this model involves again a question concerning the definition of the time scaleT^t_{SG}. What is the dependence of this time scale on the turbulence time scale (and here we mean the subgrid scale turbulence)? Is the propagation velocity of the "subgrid scale flamelet" expected to play?

The answers to these questions can follow again from the recent knowledge about turbulent flames. In the case of wrinkled flames, it is now known that the long, wrinkled, flamelet is continuously stretched by turbulence, increasing the flamelet surface area per unit of volume, and at the same time this area is decreased by the consumption of the smallest pockets, or tongues, of unburnt gases, because the classical normal propagation of flamelets. The actual flamelet surface area per unit of volume, which is directly proportional to the mean reaction rate in this volume, is the result of these two opposite tendencies. The first evidence of this has been shown using a "cellular automaton" simulating an academic constant density turbulent flame [10].

If the flamelet answer very rapidly to these two forces, there is an algebraic relationship (i.e. instantaneous and local) between this area and turbulence, including the laminar flamelet velocity of propagation. The BML formula is supposed to be this algebraic formula : then it is implied that the non-dimensional factor C_{SG} may be a function of the ratio of the (subgrid scale) turbulent kinetic energy to the square of the laminar flame velocity. In addition, the time scale is the mean subgrid scale time scale of the turbulence.

But if the flamelet does not adapt itself instantaneously, we need to use an unsteady balance equation for the evolution of the flame surface density. Such an equation has been proposed for RANS models, and can be transposed in the LES context.
We will consider here the approach of Mantel and Borghi [11], using an equation for the mean dissipation rate of the progress variable fluctuations. This quantity has been shown to be directly proportional to the mean reaction rate and to the mean flamelet surface area per unit of volume Σ :

$$\overline{\rho}\widetilde{\dot{w}}_c = \rho_u S_L \Sigma = \overline{\rho}\frac{\varepsilon_c}{1-b} \qquad (4)$$

b is a constant, smaller than one, defined in the BML theory (see [2]), that can depend again on some chemical characteristic, but not on the Damköhler number (see [3]).
With the recent improvement of Mura and Borghi [12], the modelled equation is (5) :

$$\frac{\partial}{\partial t}\left(\overline{\rho}\varepsilon_c\right)+\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}\varepsilon_c(\widetilde{v}_\alpha - U_{L\alpha})\right)=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial \varepsilon_c}{\partial x_\alpha}\right)+C_{pc}\overline{\rho}D_{SG}\frac{\varepsilon}{k}\frac{\partial\widetilde{c}}{\partial x_\alpha}\frac{\partial\widetilde{c}}{\partial x_\alpha}+C_{pu}\overline{\rho}\nu_{SG}\frac{\partial v_\alpha}{\partial x_\beta}\frac{\partial v_\alpha}{\partial x_\beta}+a\overline{\rho}\frac{\varepsilon}{k}\varepsilon_c - a'\overline{\rho}\frac{\varepsilon_c^2}{\widetilde{c}(1-\widetilde{c})}$$

$U_{L\alpha}$ is an additional velocity, discussed in [11], which becomes negligible when the turbulent kinetic energy is large with respect to the square of the laminar flame velocity. The C's and a are constants, but a' is a function of the ratio $S_L/k^{1/2}$.
This equation is very similar to equations derived for Σ directly, see [13] for instance.
Of course, here the turbulence characteristics are relative to the subgrid turbulence only.
Then a new model consists in using (2) with the mean reaction rate (the last term on the right) expressed in terms of ε_c by (4), with ε_c calculated by (5).
One see in (5) that when the last two terms are predominant, one recover an algebraic formula similar to the BML formula, with an explicit appearance of $S_L/k^{1/2}$ in the formula coming from the factor a'. Indeed, for LES approach, we can expect than the convective and diffusive terms in this equation are smaller than the similar terms for the RANS equation, while the stretching term and flamelets propagation term, that play only at small scales, are the same. It follows that the use of the algebraic BML model, i.e. directly equation (2), is probably more suited for LES than for RANS, but this depends actually of the grid size : for sufficiently small grid size, (2) is enough, but the cost of calculation could be too large…

II.3 Discussions concerning the subgrid scale eddy diffusivity

Countergradient turbulent diffusion is a well known phenomenon in turbulent premixed combustion. The discussions about this effect, as well as the proof of its experimental evidence have been proposed by K.Bray, P.Libby and B.Moss, see for instance [14], in the framework of RANS models. DNS of premixed one dimensional turbulent flames have revealed since 1990 most of the aspects of this phenomenon, in particular the recent work of Veynante et al. [15].
Can we infer, from these studies, that the classical gradient law for the subgrid scale eddy diffusivity are realistic or not? Unfortunately, the answer is that the countergradient effect is likely to occur also for subgrid scale fluxes, and consequently the classical eddy diffusivity models that have been used for non reactive flow are not well suited here.
Indeed, it has been shown that countergradient diffusion mostly occurs for flames where the turbulent kinetic energy is of the same order as the square of the laminar flame velocity, the classical gradient type turbulent diffusion being again valid when the ratio of these quantities is above two or three (depending on the density ratio between unburnt and burnt gases). This holds in the case of a turbulent flame that propagates normally to itself, or is stabilized perpendicularly to the main velocity of the flow, as in [15], [16]. When we consider LES models, the subgrid scale turbulent kinetic energy is always smaller than the full turbulent

kinetic energy, and consequently the ratio with the square of the laminar velocity is smaller. Then countergradient diffusion is more probable for LES, and even, with sufficiently small grid a countergradient diffusion model will be unavoidable. Only when the grid will be smaller than the laminar flame thickness the gradient diffusion will be recovered, and that is not at all interesting for LES.

The understanding of the countergradient effect needs to consider the balance equation for $\phi_\beta = \overline{\rho c' v'_\beta}/\overline{\rho}$, the turbulent flux of the progress variable. This equation is the same for subgrid flux as for the full flux, and it writes, with the Favre formalism :

$$\frac{\partial}{\partial t}\left(\overline{\rho}\phi_\beta\right)+\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}\phi_\beta\tilde{v}_\alpha\right)=\frac{\partial}{\partial x_\alpha}\left(-\overline{\rho c' v'_\alpha v'_\beta}\right)-\overline{\rho}\phi_\alpha\frac{\partial\tilde{v}_\beta}{\partial x_\alpha}-\overline{\rho v'_\alpha v'_\beta}\frac{\partial\tilde{c}}{\partial x_\alpha}-\overline{c'}\frac{\partial\overline{p}}{\partial x_\beta}-\overline{c'\frac{\partial p'}{\partial x_\beta}}-\chi_{c\beta}+\overline{\rho\dot{w}_c v'_\beta}$$

I II III V IV VI VII X

where $\chi_{c\beta}=\overline{v'_\beta\frac{\partial j_\alpha}{\partial x_\alpha}}+\overline{c'\frac{\partial\tau_{\alpha\beta}}{\partial x_\alpha}}$ contains two molecular dissipation terms (VIII + IX). The superscript (‘) indicates the fluctuations around the Favre mean value, except for the pressure where the fluctuations are considered around the Reynolds average.

The importance of the different terms in the equation is different in the case of gradient diffusion and in the case of countergradient, which occurs for smaller turbulent kinetic energy. In the first case, the term with the gradient of the mean c (IV) balances the correlation of c’ and the fluctuating pressure gradient (VII), the other ones being almost negligible. In the second case the situation is more complex and the molecular dissipation terms (VIII+IX) are the larger destruction term, while the pressure gradient terms (VI+VII) are the larger production terms. But the other terms are not fully negligible. Fig. 4 illustrates this finding, from [15]. On this figure, the curves show the time evolution of the spatial integration of the different terms of the scalar flux budget. Fig. 5 shows the distribution of these terms at different location within the flame brush, averaged with time during the steady propagation of the flame, calculated in [16].

The modelling of such an equation is not easy, in particular due to the term VII, which has two opposite roles … However, recent works have given realistic proposals, see [16]. The modelled equation (with D/Dt the material derivative) is (6):

$$\overline{\rho}\frac{D}{Dt}\phi_\beta=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial\phi_\beta}{\partial x_\alpha}\right)-\overline{\rho}\phi_\alpha\frac{\partial\tilde{v}_\beta}{\partial x_\alpha}-\overline{\rho v'_\alpha v'_\beta}\frac{\partial\tilde{c}}{\partial x_\alpha}-\overline{c'}\frac{\partial\overline{p}}{\partial x_\beta}-.68\overline{\rho}\frac{\phi_\beta}{T^t_{SG}}+\overline{\rho}S_L\left(\frac{\rho_u}{\rho_b}-1\right)(.5-\tilde{c})\tilde{\dot{w}}n_\beta+\overline{\rho}\frac{\phi_\beta\tilde{\dot{w}}(.7-\tilde{c})}{\tilde{c}(1-\tilde{c})}$$

The vector n_β is nothing but the unity vector normal to the mean flame brush : $n_\beta=\frac{\partial\tilde{c}}{\partial x_\beta}/\left|\nabla\tilde{c}\right|$.

The term VI is easy to calculate in the thin flamelet limit. It gives :

$$\overline{c'}\frac{\partial\overline{p}}{\partial x_\beta}=\overline{\rho}\tilde{c}(1-\tilde{c})\left(\frac{1}{\rho_b}-\frac{1}{\rho_u}\right)\frac{\partial\overline{p}}{\partial x_\beta}$$

The scalar flux itself can be calculated from this equation, and the eddy diffusivity is no more usefull in eq.(1) or (2).

For LES, we can expect, at least with sufficiently small grid size, than the source and sink terms are predominant with respect to the convection and diffusion terms. Then, an approximate algebraic formula could be obtained (neglecting also the mean velocity gradient effect) :

$$\overline{\rho}\phi_\beta\left(\frac{.68}{T^t_{SG}}-\frac{\tilde{\dot{w}}(.7-\tilde{c})}{\tilde{c}(1-\tilde{c})}\right)=-\overline{\rho v'_\alpha v'_\beta}\frac{\partial\tilde{c}}{\partial x_\alpha}-\overline{\rho}\tilde{c}(1-\tilde{c})\left(\frac{1}{\rho_b}-\frac{1}{\rho_u}\right)\frac{\partial\overline{p}}{\partial x_\beta}+\overline{\rho}S_L\left(\frac{\rho_u}{\rho_b}-1\right)(.5-\tilde{c})\tilde{\dot{w}}n_\beta$$

This formula is a kind of generalized linear form relating the flux to the different gradients or generalized forces. The second and third terms contain the non-gradient contribution. Of course, when the first term on RHS dominates, the classical gradient law is recovered. One sees on the formula that this can occur when a turbulent characteristic velocity, to which the first term is proportional, is large enough with respect to the laminar flame velocity, which appears in the last term.This formula has not yet been used in numerical calculations.

II.4 Calculation of the subgrid scale turbulent kinetic energy

The model will be completed only when the (subgrid scale) eddy diffusivity, eddy viscosity, and time scale will be given. These three quantities are linked with the subgrid scale turbulent kinetic energy (tke), and we first discuss the question of the calculation of this quantity.
For RANS models, the existence of the so called “flame generated turbulence” has been discussed since the fifties. Experimental evidence has been found, and recent DNS have been necessary in order to understand the different aspect of this question. With the classical definition of unconditioned tke, it has been shown that combustion produces tke, non isotropically, due to the differential acceleration of the light burnt gases and the heavy unburnt gases in a force field due to the pressure gradient. This effect is not simply related to the flapping of the wrinkled flamelets. The classical source of turbulence due to mean velocity gradients can also be increased by combustion and expansion of gases, and this probably dominates for oblique flames. Additional dissipation of tke occurs also, but the global result is an increase, and a very important characteristic is that the new source of turbulence is not simply linked to mean velocity gradients. These phenomena have been very clearly identified in [17] for a premixed flame that propagates normally to itself in a given turbulent flow. Fig. 6 and 7 illustrate these facts.
These phenomena hold for the total tke, but also for the subgrid scale tke. The additional source related to the pressure gradient has two parts, one related to the mean pressure gradient and one related to the fluctuating pressure gradient. The first part depends on the global geometry of the flow (open or confined) and concerns the large scales, but the second one is necessarily related to the flamelets, to which a localised pressure drop is attached. This second part is present at the scale of the flamelets thickness, then at the subgrid scale, and is more and more important in the tke budget when the grid size decreases.
The modelling of subgrid scale tke has to take this new source into account. The classical models, which take simply into account the mean (large scale) velocity gradient don’t do that.
The modelling of the described effects for tke in RANS model is based on a balance equation that includes new modelled terms. We can consider [17] or [18] for that. Following [17], the equation writes as eq. (7) :

$$\overline{\rho}\frac{D}{Dt}k=\frac{\partial}{\partial x_\alpha}(\overline{\rho}D_{SG}\frac{\partial k}{\partial x_\alpha})-\overline{\rho v'_\alpha v'_\beta}\frac{\partial \widetilde{v}_\beta}{\partial x_\alpha}-\overline{\rho}(\frac{1}{\rho_b}-\frac{1}{\rho_u})\phi_\alpha\frac{\partial \overline{p}}{\partial x_\alpha}+.35\overline{\rho}\widetilde{w}S_L^2\left(\frac{\rho_u}{\rho_b}-1\right)^2-\overline{\rho}\varepsilon-\frac{\overline{\rho}^2}{\rho_u}S_L k^{1/2}(\frac{\rho_u}{\rho_b}-1)\widetilde{w}$$

One sees the term related to the mean pressure gradient, and the new production due to the flamelets, as well as the new dissipation. The scaling of these terms is explained in [17].
The classical dissipation rate ε, in the framework of LES, has to be related to tke and the grid size Δ (linked to the spatial filter that is used for defining the mean values) :

$$\varepsilon=C_{ESG}\frac{k^{3/2}}{\Delta}$$

This expression is simply based on the assumption that the small scale part of the spectrum of turbulence displays a similar shape, at every place, at any time, in the flow. Improvements for

this assumption could be necessary, but this is the usual point of view of LES subgrid scale models.
The subgrid tke is needed for two purposes. The first classical one is related to the calculation of the subgrid eddy viscosity and diffusivity. In the well known Smagorinsky model, for instance, the eddy viscosity is proportional to a conveniently defined norm of the mean velocity gradient, and to the square of the grid size :

$$\nu_{SG} = C_{USG} \Delta^2 \left\| \nabla \tilde{V} \right\|$$

In order to take into account the fact that the tke is not simply related to the mean velocity gradient, we can adopt here the formula : $\nu_{SG} = C_{USG} k^{1/2} \Delta$, and for the eddy diffusivity : $D_{SG} = C_{DSG} k^{1/2} \Delta$. This eddy diffusivity is not used in the mean progress variable equation (2), but is again useful for the other equations (5), (6), (7).
The second need of subgrid scale tke is for expressing the subgrid time scale. Again with the assumption that the size of the grid and the subgrid scale tke suffice, on get :

$$T^t_{SG} = C_{TSG} \frac{\Delta}{k^{1/2}}$$

The proportionality constants C's are to be fixed as usual.

As for the turbulent flux of the progress variable, we can expect that the source and sink terms of the balance of tke are predominant for sufficiently small grid size, and then we could get a local algebraic formula easier to use. By inspection of the tke balance equation, we can see that not only mean velocity gradient is important now, but also two other phenomena : the reaction rate, and the mean pressure gradient. These two ingredients are not taken into account in the Smagorinsky model, and can be incorporated now.

III. Models for moderately fast chemistry;

III.1 Moderately fast chemistry has to be considered for two different purposes. The first one concerns the case when the combustion chamber is operated close to the extinction or ignition limits. Then chemical time scales cannot be considered as very small with respect to the mechanical time scales. The second case deals with the pollutant formation. The chemistry of nitrogen oxides, for instance, is much slower that combustion itself (this holds for the Zeldovitch mechanism), and the soot oxidation takes place also in the post flame zone. When chemistry is not very fast, considering wrinkled quasi-laminar flamelets in the flame brush is not sufficient for building a picture of the full phenomenon. A first, very simple, modification of the flamelet approach incorporates in the proportionality constant of (2), or in the definition of S_T in (3), the influence of the stretching of flamelets, depending on the Karlovitz number. This has been done for RANS approach in the BMLC model. In order to go further, trying to include reignition of flamelets, or their transient behavior during fast transient stretching and compression periods, a PDF approach is necessary. It is clear that the PDF approach can also be extended to subgrid scale only, in the LES methodology. The equations will be the same, the closure can be similar, but the meaning of the physical quantities will be different and their numerical value will be different…
The first question to be solved in this case consists in getting a convenient representation of the chemical mechanism and the chemical reaction rates, including a number of variables as small as possible. This question can be solved considering reduced mechanisms, or using the ILDM approach (see [19], or [3]). The second question concerns the micromixing model. It has to be emphasized here that the micromixing model can incorporate features that are related to the presence of flamelets that are perturbed by intense stretching and turbulent mixing, but do keep their reaction zone very similar to the laminar structure, see [20].

III.2 Presumed subgrid scale PDFs

Because PDF equations are quite expensive to solve, it seems interesting to consider the possibility to use “presumed shapes”, depending only of a few parameters that could be calculated at each location in the field. Then, it can be interesting to revisit the old-fashioned paper of Borghi and Moreau in 1977 [21]. Very simple shapes, built with rectangles and Direct peaks, have been proposed for a one dimensional PDF, and the calculation of the PDF was possible by knowing only at each location the mean and the variance of the fluctuations of the progress variable. For non-premixed flames, a so-called “beta function” has also be very often used for the mixture fraction PDF, see [3]. These presumed PDF shapes can evidently be used also for subgrid scale PDFs. We can even expect than these PDFs are simpler than the full ones, and simple approximations will not lead to large errors. The PDF shape is easier to presume when a single progress variable is needed, and we consider this case first.
The balance equation for the mean progress variable in moderately fast chemistry is similar to (2), but with the mean reaction rate that is calculated with the PDF:

$$\frac{\partial}{\partial t}\left(\overline{\rho}\widetilde{c}\right)+\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}\widetilde{c}\widetilde{v}_\alpha\right)=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial\widetilde{c}}{\partial x_\alpha}\right)+\overline{\rho}\int_0^1\dot{w}(c)\widetilde{P}(c)dc \qquad (8)$$

The equation for the variance of (subgrid scale) fluctuations of c is:

$$\frac{\partial}{\partial t}\left(\overline{\rho c'^2}\right)+\frac{\partial}{\partial x_\alpha}\left(\overline{\rho c'^2}\widetilde{v}_\alpha\right)=\frac{\partial}{\partial x_\alpha}\left(\overline{\rho}D_{SG}\frac{\partial(\overline{\rho c'^2}/\overline{\rho})}{\partial x_\alpha}\right)-\overline{\rho v'_\alpha c'}\frac{\partial\widetilde{c}}{\partial x_\alpha}+2\overline{\rho}\int_0^1 c'\dot{w}(c)\widetilde{P}(c)dc-\overline{\rho}\varepsilon_c$$

The reaction terms are easy to calculate when the approximate shape of the PDF is known, and this is possible, simply as a function of c with the two parameters $\widetilde{c}$ and $\overline{\rho c'^2}/\overline{\rho}$. It has to be remarked that, in the case where the variance is small and the PDF is not thickly distributed around the mean value of c, the equation (8) becomes very similar to (1). On the other hand, in case where the fluctuations of c are very large, and that can occur only when the chemistry is very fast, the equation (8) becomes exactly (2). The interested reader can find the demonstration of this in [3].
The closures assumptions for the scalar dissipation rate and for the scalar flux have to be derived from the previous discussions in section II. In the case where the chemistry is not fast, the ratio of turbulent kinetic energy and the square of the laminar flame velocity is probably large, so it is expected that the classical gradient law can be used.
The question of finding approximate shape of PDFs in case of multidimensional PDFs is more difficult. This can be necessary when the chemistry cannot be represented by a single variable, or when the premixing is not perfect or the combustor is not adiabatic… The consideration of “partial PDFs”, proposed in [22] is a step in this direction.

IV.Conclusions.

LES modelling of turbulent combustion is of interest for helping smart control of turbulent combustion. The computers are now large and fast enough to consider this type of modelling for real combustors, but DNS is not possible. The knowledge that has been gained so far for RANS models is useful for LES models. In particular it is clear that, if we want to keep the grid size realistically large, the submodels for the subgrid scale mean reaction rates are very similar to the mean reaction rate submodels for RANS. It has also to be emphasized that, for

premixed turbulent combustion, countergradient diffusion and flame generated turbulence at the subgrid scale are expected to be important. Then, submodels for subgrid scale eddy viscosity and eddy diffusivity need to take care of these phenomena. The submodels classically adopted can be very wrong in the circumstances where these phenomena are not overhelmed by the classical mechanisms. The researchers involved in this LES approach have to take care of that. A final word is also in order concerning the behavior of the LES models in the vicinity of walls. A particular care has also to be taken, because the decomposition between large eddies and small scale fluctuations is not so clear…

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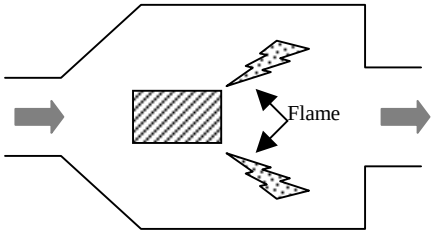

Fig. 1. Schematic drawing of the combustor.

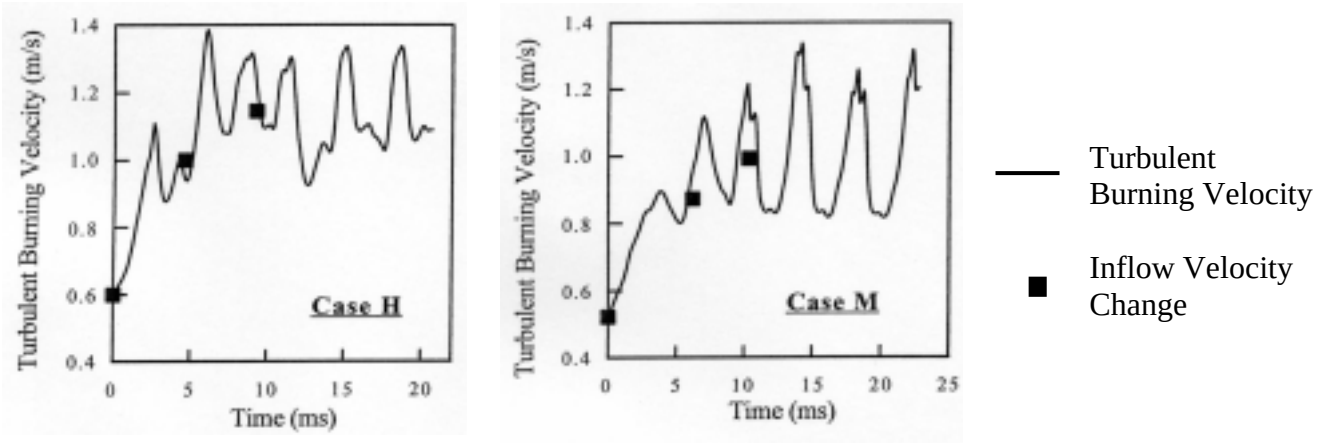

Fig. 2. Time evolution of turbulent burning velocity.

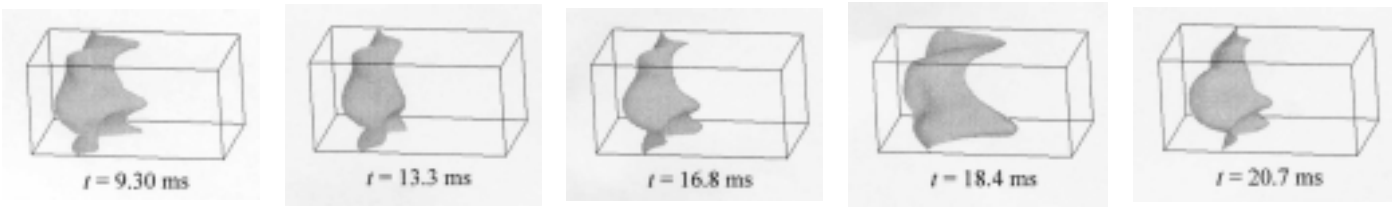

Fig. 3. Temporal evolution of wrinkled flames : contour surfaces of the progress variable at about c = 0.6. Case H (at 1470 K), from [16].

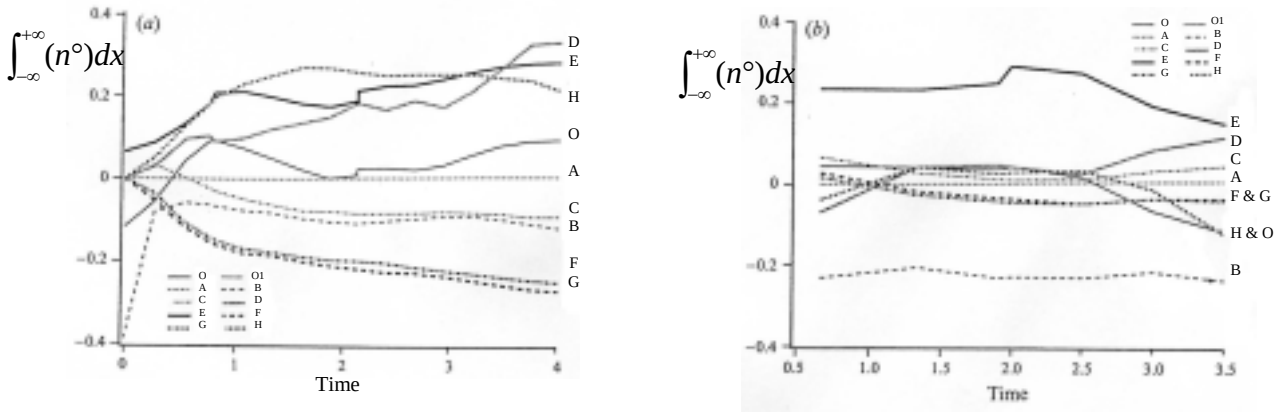

Fig. 4. Time evolution of the different terms appearing in the Φ budget, after spatial-integration over the turbulent flame brush, from [15].

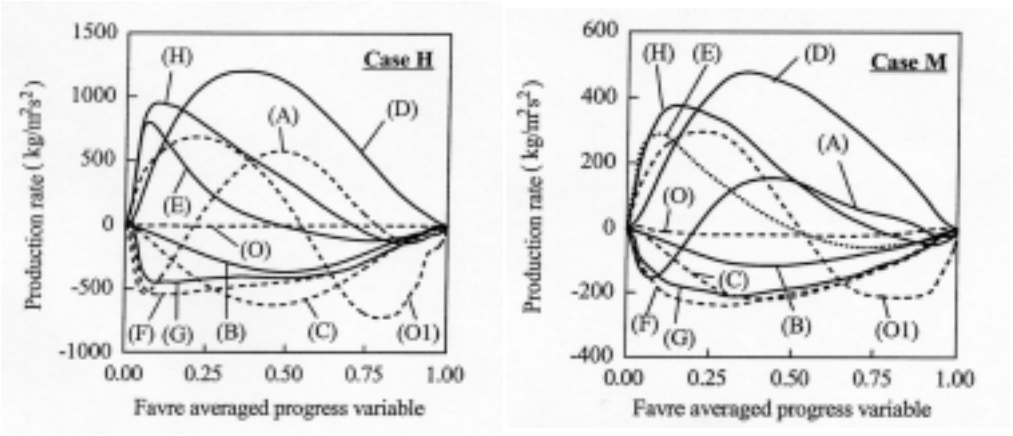

Fig. 5. Streamwise balance of the production rate of turbulent scalar flux, from [17].

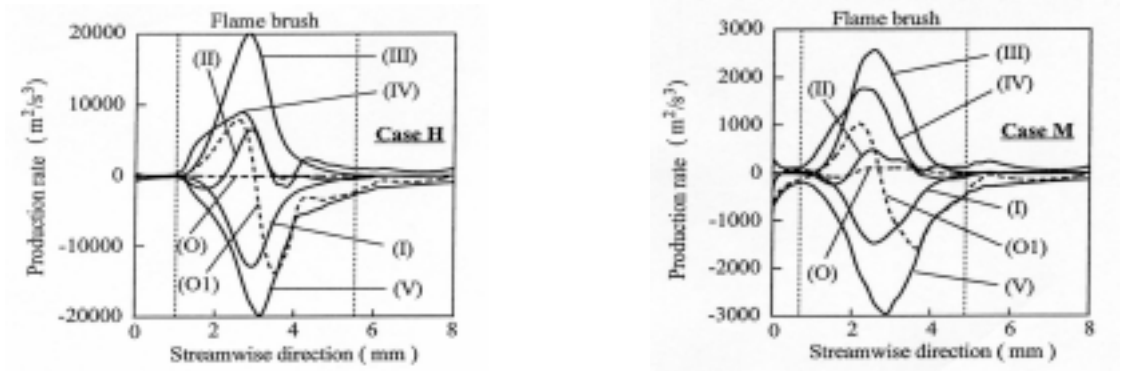

Fig. 6. Streamwise balance of the production rate of turbulent kinetic energy. The term (O) is calculated from the transport equation by substracting the convection term from the right hand side.

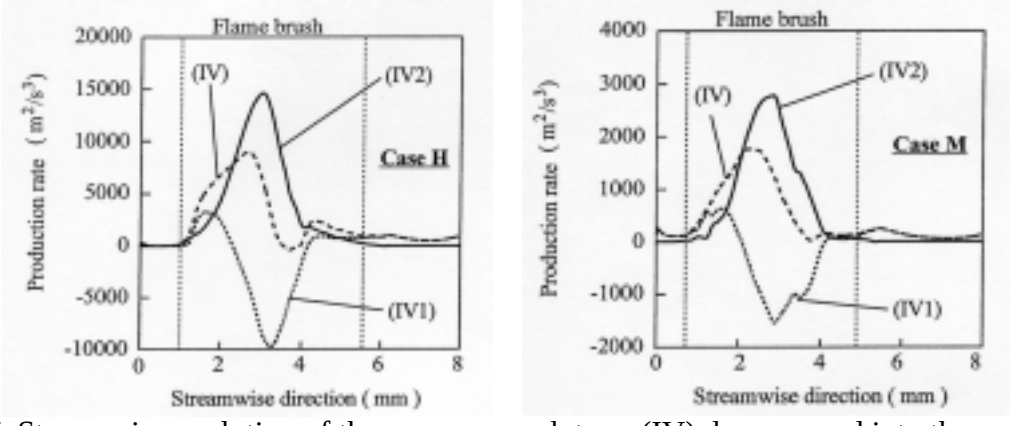

Fig. 7. Streamwise evolution of the pressure work term (IV) decomposed into the pressure diffusion term (IV1) and the pressure dilatation term (IV2), from [17].