Direct Numerical Simulation of a statistically stationary turbulent premixed flame

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1 Introduction

Premixed turbulent combustion is a common procedure in industry operating systems and in laboratory experiments. The understanding and control of interaction between the turbulence and the flame are important issues when optimizing combustion processes to comply with economical and ecological requirements. Accurate numerical simulations of such devices have to reproduce the whole characteristics of the flow. However, despite the tremendous increase of the performances of calculators, it is still non possible to resolve numerically all the turbulent scales for industrial devices geometries. Therefore averaged flow equations are solved where several unclosed terms appear depending on the averaging method retained : filtering (LES) or Reynolds averaging (RANS).

Direct numerical simulation (DNS) appears as an efficient tool to develop models and has been widely used in premixed combustion [1]. But, in most of the previous studies, a planar premixed flame is wrinkled by isotropic homogeneous turbulence (turbulence is decaying in time), whereas in industrial and experimental situations the flame encounters a spatially decaying turbulence [2, 3] (ie grid turbulence).

The aim of this work is to realize DNS of a stabilized planar premixed flame in a spatially decaying turbulence. Attention is confined to premixed turbulent combustion burning in the laminar flamelet regime [4]. This is a classic configuration for Low Mach Number formulation [5, 6], however, in those cases, pressure effects are neglected whereas they may be of great importance. Therefore, a new method has been developed for fully compressible subsonic flows [7].

Finally, a close look has been given to the modeled expressions for the terms involving pressure gradients in second moment turbulence models of premixed combustion derived by Domingo and Bray [8].

2 Presentation of the DNS data base

The simulation has been performed using a fully compressible DNS code with a single-step Arrhenius law. To decrease the cpu cost, a two dimensional simulation has been retained. To initialize the simulation, a stabilized planar premixed flame is computed. The boundary conditions are periodic in the direction parallel to the flame surface and are non reflective outflow boundaries at the outlet. A new method has been used to simulate the incoming turbulence. A spectral code is coupled to the sixth order central finite difference code to predict velocity and pressure at the inlet of the domain. In the spectral code, a forced [9] homogeneous isotropic turbulence (Passo-Pouquet spectrum) with prescribed properties is simulated. Appropriate multidimensional boundary conditions have been implemented to avoid numerical acoustic waves in the finite difference code. The figure 1 presents the vorticity on both domains : the spectral area where the turbulence is forced and the DNS area where the fully compressible equations are solved.

The mesh for the spectral code is 512*512 points and 1024*1024 for the finite difference code. At inlet of the second domain, parameters are : $(2/3\tilde{k})^{1/2}/S_L = 2$, $L_t/\delta_l = 30$, $Re_t = 81$ and $\tau = 2$ where S_L is the laminar flame velocity, L_t is the integral scale, δ_l the laminar flame thickness defined by $\delta_l = (T_{burnt} - T_{unburnt})/(dT/dx)_{max}$, τ the heat release parameter and k the kinetic energy.

A turbulent flame is obtained where the thin reactive zone is strained and curved by the vorticity of the spatially decaying turbulence (Fig : 1). In this regime of combustion, pockets of fresh gases may cross the flame surface. The fluctuations of the flame speed (Fig : 1 : bottom right) are due to this pockets crossing the flame surface. After five eddy turn over time, the flame properties are statistically stationary (Fig : 1 : bottom right).

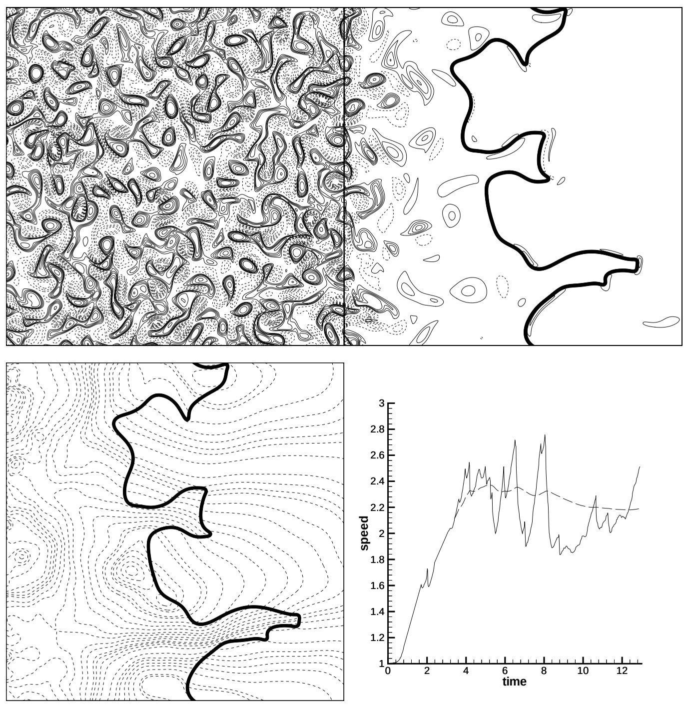

Figure 1: Top : spectral and DNS code, thick line : reaction rate, thin and dashed lines : vorticity. Left bottom : thick line : reaction rate, dashed lines : pressure field. Right bottom : thin line : turbulent flame speed nondimensionalized using S_L versus eddy turn over time , dashed line : average flame speed.

The figure 2 shows the Karlovitz number (Ka) along streamwise direction. Ka decreases in space and is close to 0.2 in the region where the flame is found. According to the Klimov-Williams criterion, the combustion is then strictly in the laminar flamelet regime.

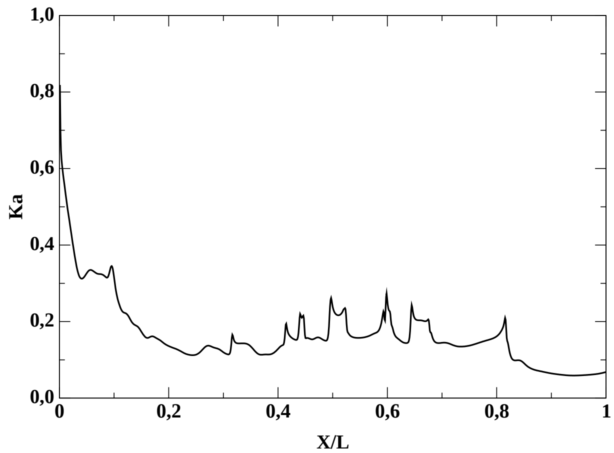

Figure 2: Karlovitz number along X_1 direction.

3 Models and discussion

In the thin flamelet combustion regime the probability density function of the progress variable c is strongly bimodal. The BML formalism [10] leads to the following expression : $\widetilde{u_i'' c''} = \tilde{c}\,(1-\tilde{c})\,(\bar{u}_{iP} - \bar{u}_{iR})$ where u_i is the flow velocity , subscripts R, P, F represent the conditional mean contribution from reactants, products and flamelet respectively, $\widetilde{()}$ the Favre average and $\bar{()}$ the Reynolds average.

In second moment models for turbulent flow, closure of the averaged flow equations is achieved by solving a transport equation for each component of the Reynolds stress and the Reynolds flux. The terms of present interest in these two equations are the terms containing the pressure gradient : $\overline{u_j'' \frac{\partial p}{\partial x_i}}$ and $\overline{c'' \frac{\partial p}{\partial x_i}}$

The models proposed for these terms [8] are applicable to the thin laminar flamelet regime of premixed turbulent combustion. They are based on a systematic partitioning of each covariance into contributions from reactants, products and flamelets. The pressure gradient covariance terms are then given by :

$$
\begin{aligned}
\overline{c'' \frac{\partial p}{\partial x_k}} &= \frac{\tilde{c}\,(1-\tilde{c})}{1+\tau\tilde{c}} \left((1+\tau)\,\frac{\partial \bar{p}_P}{\partial x_k} - \frac{\partial \bar{p}_R}{\partial x_k} \right) + \frac{\tau}{2} < n.N_k > \bar{\sum}_F \rho_R S_L^2\,(0.7-\tilde{c}) \\
\overline{u_j'' \frac{\partial p}{\partial x_k}} &= \frac{\widetilde{u_j'' c''}}{1+\tau\tilde{c}} \left(-\frac{\partial \bar{p}_R}{\partial x_k} + (1+\tau)\,\frac{\partial \bar{p}_P}{\partial x_k} \right) + \frac{1-\tilde{c}}{1+\tau\tilde{c}} \left(\overline{u_{R_j'} \frac{\partial p_R'}{\partial x_k}} \right)_R \\
&+ \frac{(1+\tau)\,\tilde{c}}{1+\tau\tilde{c}} \left(\overline{u_{P_j'} \frac{\partial p_P'}{\partial x_k}} \right)_P - \frac{1}{2} \bar{\sum}_F \rho_R \tau S_L^2 < n.N_k > \frac{\widetilde{u_j'' c''}}{(1-\tilde{c})} \\
&- \frac{0.7}{2} \bar{\sum}_F \rho_R \tau^2 S_L^3 < (n.N_j)(n.N_k) >
\end{aligned}
$$

where p is the pressure, ρ the density, $< n.N_k >$ and $< (n.N_j)(n.N_k) >$ are geometric parameters, $()'$ and $()''$ are respectively Reynolds and Favre fluctuations. These closures appear to do well when compared to 2D DNS in freely decaying turbulence [8].

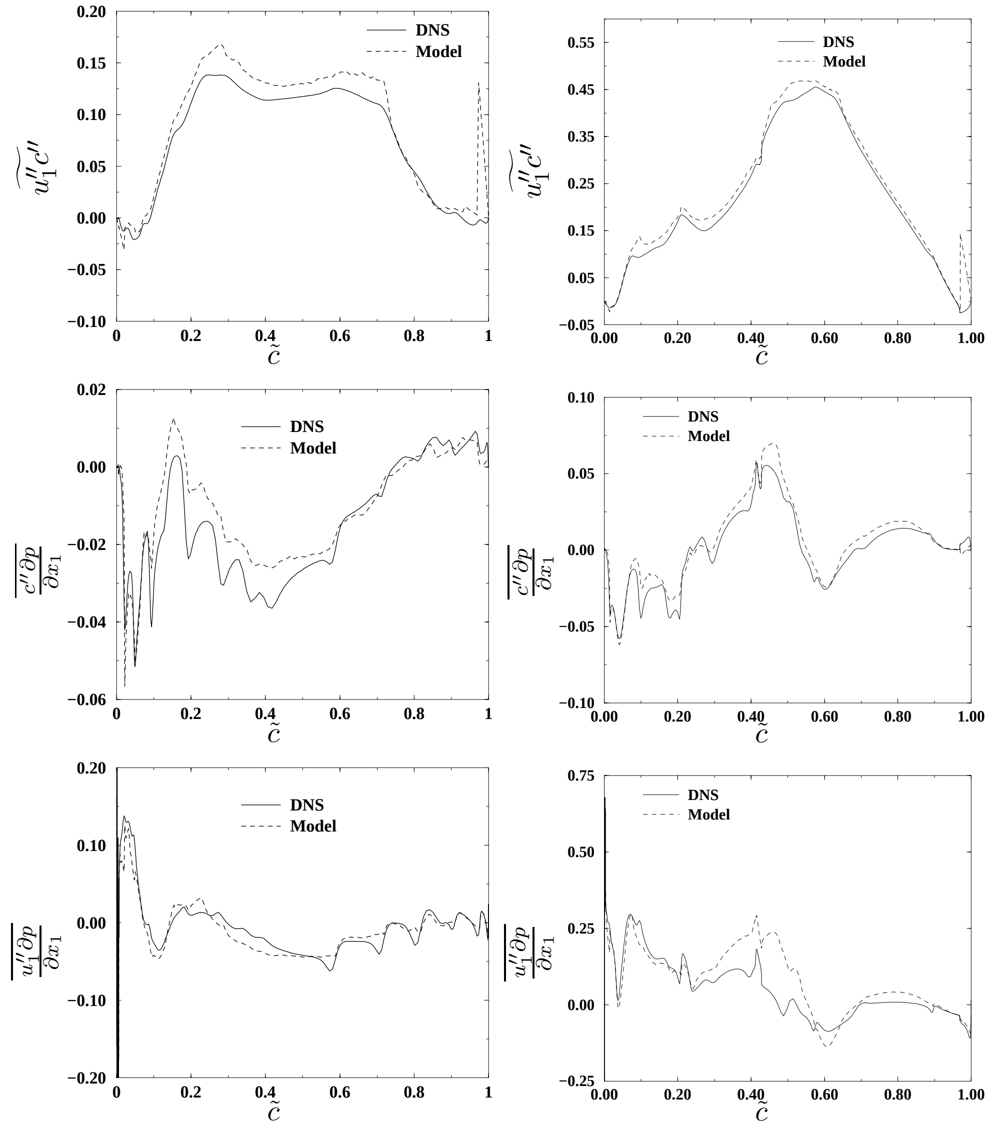

Figure 3: Left column : data at 2.5 eddy turn over time. Right column : data at 11 eddy turn over time. Top : Turbulent $\widetilde{c}$-flux plotted versus Favre mean progress reaction variable. Middle : $\overline{c'' \frac{\partial p}{\partial x_1}}$ versus Favre mean progress reaction variable. Bottom : $\overline{u_1'' \frac{\partial p}{\partial x_1}}$ versus Favre mean progress reaction variable.

Models and DNS data are displayed on the figure 3. Data are presented for two eddy turn over time. The turbulent fluxes show that the flame is dominated by countergradient diffusion of $\widetilde{c}$. Model for these fluxes is well verified. This is a consequence of the fact that for this simulation the pdf of the progress variable c is fully bimodal. The models for $\overline{u_j'' \frac{\partial p}{\partial x_i}}$ and $\overline{c'' \frac{\partial p}{\partial x_i}}$ compare well with data from DNS. Because of severe computational constraints, the Reynolds number and the heat release of the simulation are both smaller than might ideally be desired. But model terms are all proportional to powers of τ and this consideration leads to the conclusion that the models should provide good predictions under experimental conditions. This conclusion is confirmed by the recent BML study of Bray et al. [11], which successfully used present models to predict second moment quantities in premixed turbulent flames near stagnation points.

4 Conclusion

A new numerical procedure has been used to stabilize a premixed flame in a spatially decaying turbulence with fully compressible DNS code. Statistical properties of the flow are stabilized and controlled.

This configuration gives a good insight into the interaction between flames and turbulence. The models for the mean progress variable fluctuation-pressure gradient and the velocity fluctuation-pressure gradient covariances compare well with the data from DNS.

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