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High-Order Methods for the Numerical Simulation of Vortical and Turbulent Flows

DNS of premixed turbulent V-flame: coupling spectral and finite difference methods

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Abstract

To allow for a reliable examination of the interaction between velocity fluctuations, acoustics and combustion, a novel numerical procedure is discussed in which a spectral solution of the Navier–Stokes equations is directly associated to a high-order finite difference fully compressible DNS solver (sixth order PADE). Using this combination of high-order solvers with accurate boundary conditions, simulations have been performed where a turbulent premixed V-shape flame develops in grid turbulence. In the light of the DNS results, a sub-model for premixed turbulent combustion is analyzed. ***To cite this article: R. Hauguel et al., C. R. Mecanique 333 (2005).***

Résumé

Simulation directe d'une flamme en V : combinaison de méthodes spectrale et différences finies. Une nouvelle procédure numérique est discutée qui permet d'étudier de façon réaliste, l'interaction entre les fluctuations de vitesse, l'acoustique et la combustion. Dans cette approche, une solution spectrale des équations de Navier–Stokes produit la condition d'entrée d'un code de résolution des équations de Navier–Stokes pleinement compressibles. Une méthode de différences finies d'ordre élevée (schéma PADE) est utilisée dans ce deuxième solveur. En utilisant cette combinaison de solveurs avec des conditions aux limites précises, des simulations ont été effectuées dans lesquelles une flamme en V se développe dans une turbulence de grille. L'analyse de la base de données permet de comprendre le comportement de la flamme turbulente. Une fermeture est proposée pour la modélisation du micro-mélange turbulent. ***Pour citer cet article : R. Hauguel et al., C. R. Mecanique 333 (2005).***

Keywords: Fluid mechanics; Turbulent combustion; Direct numerical simulation

Mots-clés : Mécanique des fluides ; Combustion turbulente ; Simulation numérique directe

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1. Introduction

Direct numerical simulation (DNS) has been widely used to improve turbulent combustion modelling. Reynolds Average Navier–Stokes (RANS) calculation and Large Eddy Simulation (LES) of turbulent combustion motivate questions that may be addressed using Direct Numerical Simulation (DNS), where all the scales of the problem are fully resolved, at least in terms of scalar and velocity fluctuations, and where the chemical kinetics is often reduced [1–3]. Until recently, DNS was restricted to very low Reynolds number flows. Today, the status of DNS is progressively evolving with the speed-up of computers and direct numerical simulations of laboratory jet-flame experiments have even been reported with realistic chemical kinetics [4].

DNS of a premixed turbulent V-flame anchored on a hot wire is discussed in this article. To allow for a reliable examination of the interaction between velocity fluctuations, acoustics and combustion, a novel numerical procedure is used in which a spectral solution of the Navier–Stokes equations is directly coupled to a high-order finite difference fully compressible DNS solver (sixth order PADE) [5]. Using this combination of high-order solvers with a set of accurate boundary conditions, simulations have been performed where a premixed turbulent V-shape flame develops in grid turbulence. The chemistry is described with tabulated fully detailed kinetics. Flames are then analyzed in a turbulence featuring constant mean properties at any given streamwise position. The DNS is probed to propose a closure for premixed turbulent combustion, in which the FPI (Flame Prolongation of Intrinsic low Dimensional Manifold) chemistry tabulation is introduced [6].

2. Flow configuration and numerics

V-shape flames are observed when a premixed flame is stabilized on a hot wire. The combustion is initiated by the energy released by the wire on which the flame is anchored. In a laminar flow, the reaction layer propagates against the incoming fluid and a premixed V-shape flame develops. When the flow is turbulent, the two wings of the flame are wrinkled by velocity fluctuations and a turbulent flame having a V-shape, in mean, is observed. This configuration is of interest because grid turbulence may easily be generated in the incoming flow, so that combustion develops in a well characterized spatially decaying turbulence. Recent progress makes it possible to consider this configuration with DNS.

So far, fully compressible combustion DNS has been restricted to turbulence freely decaying in time [7,8]. Attempts to simulate decaying grid turbulence in DNS have already been performed in the framework of the low Mach number formalism [9]. This low Mach number approach is avoided in this work since we want to have access to information on flame acoustics. Specifically for subsonic combustion, the use of any forcing based on a synthetic random phase, generates spurious pressure oscillations that strongly perturb the flame behavior. To overcome this difficulty, two separate Navier–Stokes solvers are combined so that the incoming grid-turbulence is exactly simulated in time [10]. A DNS spectral solver and a finite difference spatial solver evolve simultaneously in time. The spectral solution is used to generate a forced synthetic grid-turbulence that continuously enters the finite difference domain, with a Galilean transformation applied to ensure the coupling between the solvers.

Fig. 1 shows the computational domains: on the left, the turbulence is forced in the spectral solution; on the right, a premixed turbulent V-flame develops in the spatially freely decaying turbulence. The forced turbulence entering the domain is thus a solution of the Navier–Stokes equations.

To accurately compute the pressure field, the NSCBC boundary conditions [11] have been coupled with the forced turbulence. The time derivative of the velocity field is explicitly introduced in the calculation of the amplitude of the acoustic waves entering the domain.

Two representative simulations have been performed where the integral turbulence scale is 10 times the characteristic flame thickness (Fig. 2). In case (a), the ratio between the characteristic velocity fluctuations and the laminar flame speed is of the order of 1.25, while it is of the order of 2.5 in case (b). The turbulent Reynolds number is 18 in case (a) and 37 in case (b). The velocity ratio is representative of values measured in V-flame experiments, but

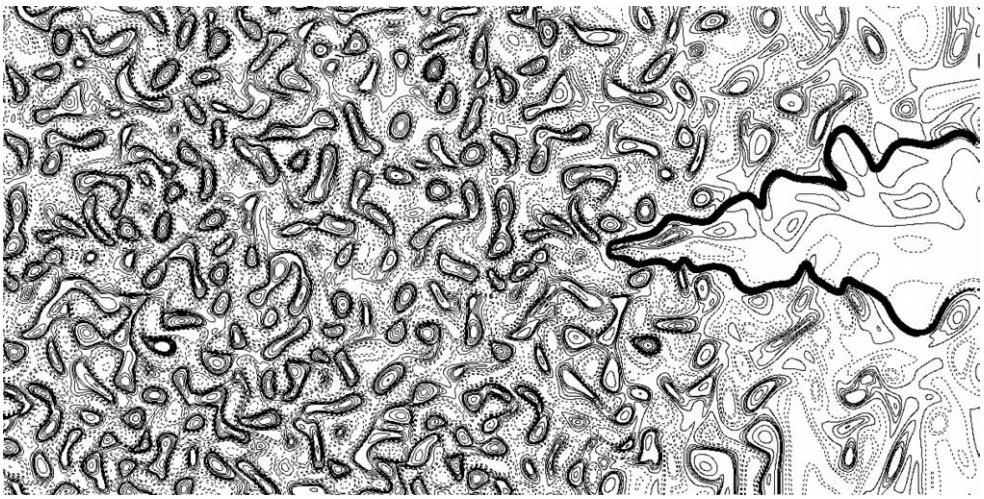

Fig. 1. Snapshots of a methane–air V-flame. Thin lines: positive vorticity, thin lines (dashed): negative vorticity, thick line: reaction rate.

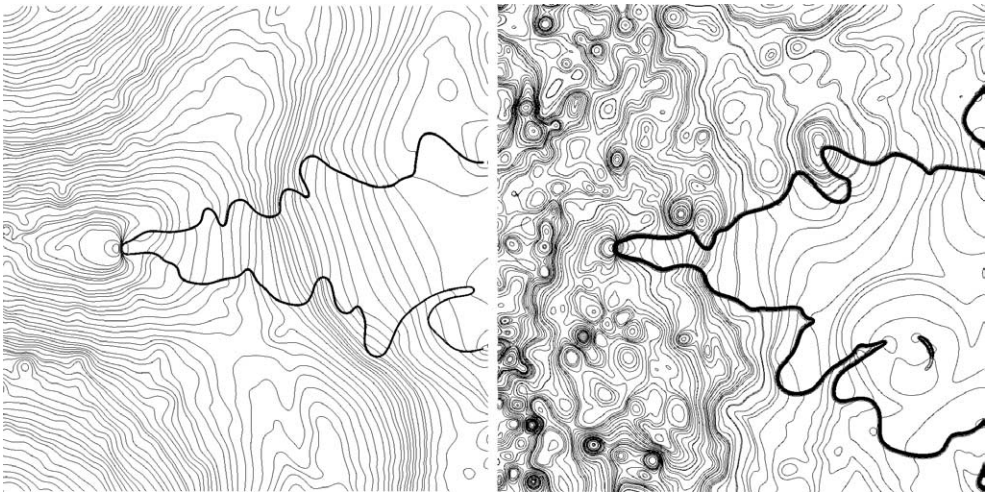

Fig. 2. Pressure field (line) and reaction rate (bold), left: case (a), right: case (b).

the ratio of length scales is an order of magnitude smaller that found in real flames. Two-dimensional simulations are performed. Theoretically, all DNS of turbulent flows should be three-dimensional; nevertheless, it was shown that most features of premixed flame turbulence interaction are found in two-dimensional DNS, as a result of the typical behavior of premixed flame surfaces when they interact with vorticity [12]. In the two-dimensional simulations reported in this article, the forced turbulence is computed on a 512×512 mesh (spectral), while the flame requires a 1024×1024 grid for case (a) and 1024×2048 in case (b) (finite difference). Since, it is not possible to introduce a wire in our solver, its effect is reproduced by imposing chemical equilibrium on a small region of the domain. The flame-turbulence interaction is not affected by the forcing scheme and the acoustic field is free from any unphysical perturbations. In particular, the local pressure drops expected in the zone bordering edge-flames are well captured (Fig. 2).

Complex chemistry is included in the solver with the FPI approach [6,13]. The detailed methane–air GRI mechanism [14] is retained to construct the FPI table for the simulations presented in this article.

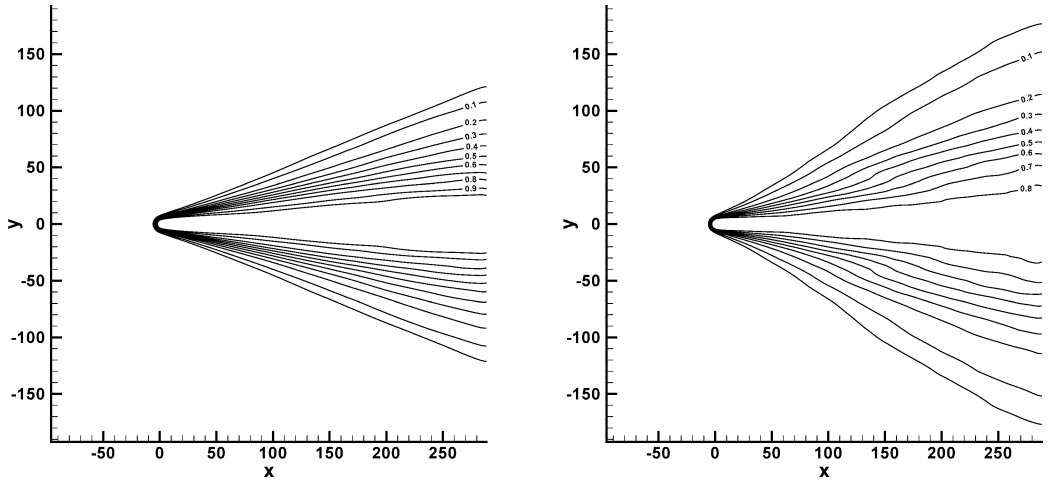

Fig. 3. Field of mean progress variable for cases (a) and (b); left: case (a), right: case (b).

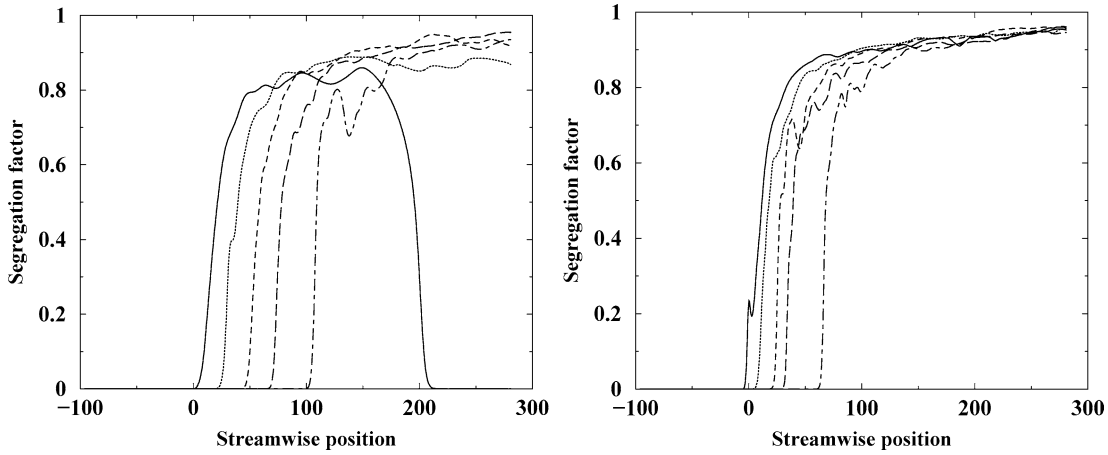

Fig. 4. Streamwise evolution of the unmixedness $S = \widetilde{c''^2}/(\tilde{c}(1-\tilde{c}))$ for cases (a) and (b). Line: $y = 11.6$, dotted line: $y = 23.6$, dashed line: $y = 35.7$, long dashed: $y = 47.7$, dot-dashed: $y = 71.7$. Left: case (a), right: case (b).

3. Flame analysis

The mean fields of the progress variable, c, are presented in Fig. 3, the generic V-shape flame is observed. This allows one to verify that the simulations are indeed stationary in mean.

The maximum level of fluctuations of progress variable is obtained when c features a telegraphic signal that is representative of a fully segregated flow, which is mostly composed of separated fresh and burnt gases [15], then $\widetilde{c''^2}_{\mathrm{Max}} = \tilde{c}(1-\tilde{c})$. Fig. 4 shows $S = \widetilde{c''^2}/(\tilde{c}(1-\tilde{c}))$, the unmixedness between fresh and burnt gases. Downstream of the stabilizing wire, S is larger than 0.8 indicating a very thin local and instantaneous reacting front and then $\widetilde{P}(c^*; \underline{x}, t)$, the probability density function (pdf) of c, takes an almost bimodal shape. The statistical properties of the internal flame structure, including pollutant formation, is then controlled by the small values of $\widetilde{P}(c^*; \underline{x}, t)$ found when c^* is between zero and unity, therefore within the thin reaction zones.

4. Accounting for flame length scales in micromixing modelling

The chemical reactions occur at the dissipative scales of the turbulent motion, where molecular diffusion is acting to bring species into contact. Both LES and RANS face the same difficulty: the unresolved small scale diffusion needs to be modeled and it is of fundamental importance for estimating the mean, or the subgrid, burning rate. When D is a representative diffusion coefficient, a characteristic mixing speed may be defined as $V_d = D|\nabla c|$. It is a measure of the speed at which the information diffuses across the local flame front of thickness $l_d = |\nabla c|^{-1}$. The ratio $\chi_c = V_d/l_d = D|\nabla c|^2$ is the inverse of a time scale, usually called scalar dissipation rate, whose average $\bar{\rho}\tilde{\chi}_c = \overline{\rho D|\nabla c|^2}$ is the stumbling block of any turbulent combustion modeling approach [16].

In the FPI context, where species mass fractions are available in the form $Y_i(c)$, when the pdf of c is known, any mean quantity is then readily obtained:

$$\widetilde{Y}_i(\underline{x}, t) = \int_c Y_i(c^*)\widetilde{P}(c^*; \underline{x}, t)\,\mathrm{d}c^* \tag{1}$$

This relation is valid for both RANS and LES, in the latter, $\widetilde{P}(c^*)$ would denote a subgrid-pdf [17]. This pdf may either be calculated or presumed, for instance via a beta-function. In both cases, turbulent micro-mixing mechanisms need to be estimated.

Basic closures for $\tilde{\chi}_c$ may be obtained from an eddy-break up type hypothesis, then $\tilde{\chi}_c = \widetilde{c''^2}/\tau_\chi$, with τ_χ a characteristic time scale that is usually estimated from a turbulence cascade time, $\tau_\chi = C_\chi \tilde{k}/\tilde{\epsilon}$, where $\tilde{k}$ and $\tilde{\epsilon}$ denote the kinetic turbulent energy and its dissipation rate. C_χ is a modeling constant. This linear relaxation is also sometimes generalized to the conditional value of diffusion, in the form of a LMSE or IEM micro-mixing modeling, widely used in pdf methods [18]; thus $(\overline{\nabla \cdot (\rho D \nabla c)|c^*}) \approx \bar{\rho}(\tilde{c} - c^*)/\tau_\chi$. More elaborate closures exist, but to illustrate the difficulty of accounting for the impact of thin reaction zone gradient in micro-mixing modeling, a direct test of the simple closure $\tilde{\chi}_c = C_\chi \widetilde{c''^2}/(\tilde{k}/\tilde{\epsilon})$ is proposed in Fig. 5, where C_χ is set to unity. To reproduce the DNS data, it is seen that C_χ needs to vary not only from case (a) to case (b), therefore with the turbulence and flame characteristics, but also across the mean flame structure. In RANS, a first alternative consists in solving a balance equation for $\tilde{\chi}_c$ [19]. This difficulty to estimate micro-scale diffusion is well documented in the literature and already observed in frozen flow mixing. In premixed combustion, molecular diffusion and chemical reaction are coupled to ensure flame propagation. Then, $\rho S_l(c)|\nabla c| = \nabla \cdot (\rho D \nabla c) + \dot{\omega}_c$, where $\dot{\omega}_c$ is the burning rate and $S_l(c)$

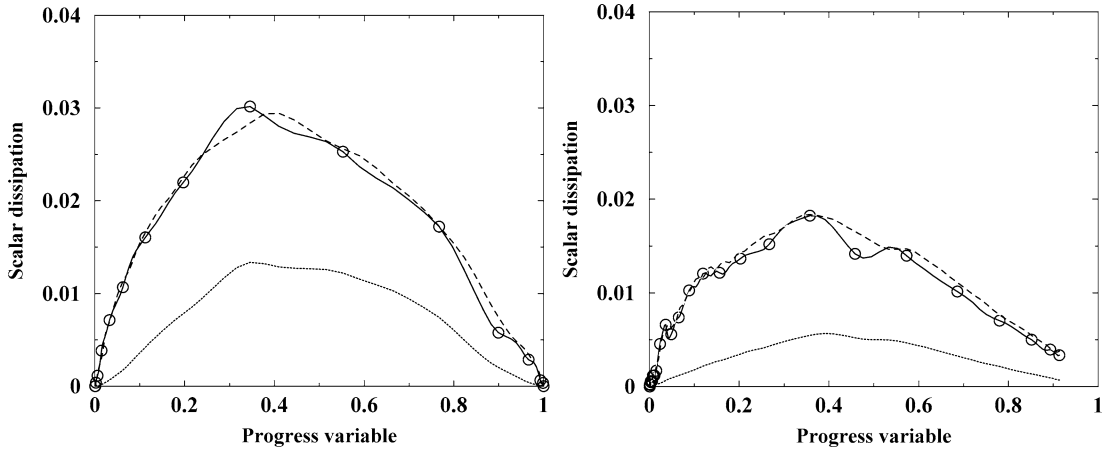

Fig. 5. Transverse distribution at $x = 47.7$ of the scalar dissipation rate $\bar{\rho}\tilde{\chi}_c$ plotted versus mean progress variable in cases (a) and (b). Line with circle: DNS. Dotted line: $\tilde{\chi}_c \approx \widetilde{c''^2}/(\tilde{k}/\tilde{\epsilon})$. Dashed line: Eq. (9).

the relative progression velocity of the iso-c surfaces. In an unstrained and planar laminar flame, $S_l(c=0) = S_l^0$ is the so-called laminar flame burning velocity. Notice, however, that $S_l(c=0)$ may differ from S_l^0 because of strain and curvature.

To help in the modeling of premixed combustion, the physical decomposition of the scalar dissipation rate in characteristic speed and length may be recovered after introducing a gradient weighted, or surface, average: $\langle a \rangle_s = \overline{a|\nabla c|}/\overline{|\nabla c|}$ [16]. Then,

$$\bar{\rho}\tilde{\chi}_c = \overline{\rho D|\nabla c|^2} = \langle \rho D|\nabla c| \rangle_s \overline{|\nabla c|} \tag{2}$$

The average turbulent speed of mixing thus appears in the form $\langle \rho D|\nabla c| \rangle_s$. The other contribution, $\overline{|\nabla c|}$, contains information on the wrinkling of the flame front. $\overline{|\nabla c|}$ is in fact the integral of the flame surface density function, $\Sigma(c^*) = (\overline{|\nabla c||c^*}) \overline{P}(c^*)$ [20], across the flame front:

$$\overline{|\nabla c|} = \int_c \Sigma(c^*)\,\mathrm{d}c^* = \overline{\Sigma} \tag{3}$$

$\overline{\Sigma} = \overline{|\nabla c|}$ is a well known quantity that has been used in RANS and LES of premixed turbulent flames in the CFM (Coherent Flame Model) [21]. The major advantage of Eq. (2) is to explicitly introduce a flame wrinkling length scale in the estimation of the scalar dissipation rate.

If the flame is able to promote propagation at the scale of the instantaneous thin interface between fresh and burnt gases, $\langle \rho D|\nabla c| \rangle_s$ is expected to be proportional to $\rho_o S_l^o$, where ρ_o is the density in the fresh gases. To seek out the exact form of $\langle \rho D|\nabla c| \rangle_s$, it is interesting to decompose the burning rate as:

$$\overline{\dot{\omega}}_c = \left\langle \frac{\dot{\omega}_c}{|\nabla c|} \right\rangle_s \overline{|\nabla c|} = \frac{\langle \dot{\omega}_c/|\nabla c| \rangle_s}{\langle \rho D|\nabla c| \rangle_s} \bar{\rho}\tilde{\chi}_c \tag{4}$$

After integrating over thin reaction zones [16], the BML analysis [22] is recovered and the ratio of surface averages of Eq. (4) is readily estimated:

$$\frac{\langle \dot{\omega}_c/|\nabla c| \rangle_s}{\langle \rho D|\nabla c| \rangle_s} = \frac{2}{2c_m - 1} \tag{5}$$

where

$$c_m = \frac{\int_c c^* \dot{\omega}_c(c^*) \overline{P}(c^*)\,\mathrm{d}c^*}{\int_c \dot{\omega}_c(c^*) \overline{P}(c^*)\,\mathrm{d}c^*} \tag{6}$$

Another estimation of the unknown burning rate may also be obtained from $\overline{|\nabla c|}$ [21]:

$$\overline{\dot{\omega}}_c = \rho_o S_l^o \overline{|\nabla c|} = \rho_o S_l^o \overline{\Sigma} \tag{7}$$

Combining Eq. (2) with Eqs. (4), (5) and (7) leads to:

$$\langle \rho D|\nabla c| \rangle_s = \frac{1}{2}(2c_m - 1)\rho_o S_l^o \tag{8}$$

where $\langle \rho D|\nabla c| \rangle_s$ appears to depend on the laminar flame speed and on the impact of turbulence on the internal flame structure via c_m. The scalar dissipation rate may then be expressed in the form:

$$\bar{\rho}\tilde{\chi}_c = \overline{\rho D|\nabla c|^2} = \frac{1}{2}(2c_m - 1)\rho_o S_l^o \overline{\Sigma} \tag{9}$$

This last expression combines a turbulent flame wrinkling length, $\overline{\Sigma}$, with the flame speed to estimate $\tilde{\chi}_c$. It is tested in Fig. 5 against the DNS results, when the c_m coefficient is calculated from Eq. (6) using a beta-pdf presumed from first and second order moment of the progress variable, the FPI tabulated chemistry provides $\dot{\omega}_c(c^*)$. An interesting

agreement is observed between the approximated scalar dissipation rate and DNS. For those DNS, c_m stays close to its expected BML value, $c_m \approx 3/4$ [22].

These results suggest a simple closure associating pdf and flame surface density, in which the balance equations for the two first moments $\tilde{c}$ and $\widetilde{c''^2}$ are considered to presume $\widetilde{P}(c^*)$. In those equations, the chemical sources, are obtained from FPI ($\dot{\omega}_c(c^*)$) and the pdf $\widetilde{P}(c^*)$:

$$\widetilde{\dot{\omega}}_c = \int_c \dot{\omega}_c(c^*)\,\widetilde{P}(c^*)\,\mathrm{d}c^* \tag{10}$$

$$\widetilde{c''\dot{\omega}_c} = \int_c (c^* - \tilde{c})\dot{\omega}(c^*)\,\widetilde{P}(c^*)\,\mathrm{d}c^* \tag{11}$$

The scalar dissipation rate entering the balance equation for $\widetilde{c''^2}$ may then be calculated from Eq. (9), ensuring a coupling between propagating thin reaction zones and turbulent mixing. All the knowledge available from flame surface density modelling can then be introduced in the closure for micromixing in order to estimate concentrations of intermediate species and pollutants.

5. Summary

A novel method allowing the reproducion of a spacially decaying grid turbulence in DNS of fully compressible flows, has been employed to study a V-shape flame. The data base generated is stationary in mean and can be used to obtain reliable results to assist RANS and LES developments. From the DNS results, a strategy is proposed to introduce flame length scales as an ingredient of turbulent micro-mixing modelling.

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