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Turbulent Flame Visualization Using Direct Numerical Simulation

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Abstract : Combustion phenomena are of high scientific and technological interest, in particular for energy generation and transportation systems. Direct Numerical Simulations (DNS) have become an essential and well established research tool to investigate the structure of turbulent flames, since they do not rely on any approximate turbulence models. In this work two complementary DNS codes are employed to investigate different types of fuels and flame configurations. The code π^3 is a 3-dimensional DNS code using a low-Mach number approximation. Chemistry is described through a tabulation, using two coordinates to enter a database constructed for example with 29 species and 141 reactions for methane combustion. It is used here to investigate the growth of a turbulent premixed flame in a methane-air mixture (Case 1). The second code, *Sider* is an explicit three-dimensional DNS code solving the fully compressible reactive Navier-Stokes equations, where the chemical processes are computed using a complete reaction scheme, taking into account accurate diffusion properties. It is used here to compute a hydrogen/air turbulent diffusion flame (Case 2), considering 9 chemical species and 38 chemical reactions.

For Case 1, a perfectly spherical laminar flame kernel is initialized at the center of a cubic domain at zero velocity. A field of synthetic homogeneous isotropic turbulence is then superposed and the turbulent flow and the flame can begin to interact. Various species can be used as an indicator for the flame front in a combustion process. Among them, the isosurface of species CO_2 at a mass fraction of 0.03 is retained here, since this value corresponds to the steepest temperature gradient in the associated one-dimensional laminar premixed flame. The results obtained have been post processed in order to study the interesting aspects of the coupling between flame kernel evolution and turbulence, such as straining and curvature impact on the flame surface area and local thickness.

For Case 2, the instantaneous structure of a non-premixed hydrogen/air flame evolving in a turbulent flow and starting from an initially planar structure is investigated. Here again, the properties of the resulting turbulent flame are of high interest and will be visualized, defining the flame front in a classical manner for non-premixed combustion using a mixture fraction isosurface. Considering the context of this publication, the emphasis is clearly set on the post-processing and visualization of the DNS data, not on the fundamental issues associated with turbulent combustion.

Keywords : Direct Numerical Simulation, Turbulent Flames, Visualization, Post-Processing.

1. Introduction

The ignition and initial development of a flame inside a turbulent flow is a problem of great interest, both from a fundamental (complex, multi-scale, fully coupled physical process) and from a practical (internal combustion engines, gas turbines re-ignition, security issues . . .) point of view. In recent years, numerical studies have become increasingly useful to understand such complex processes. In particular, Direct Numerical Simulations (DNS) have been known for over 10 years now to be ideally suited to investigate turbulent flames (Poinsot, 1996; Cant, 1999), because they do not require any particular assumption concerning the turbulence. Nevertheless, due to the huge cost of DNS, strong hypotheses have often been introduced to reduce the requested computing times (Poinsot, 1996). Furthermore, DNS are associated with complex post-processing and visualization issues, due to the extremely large quantity of raw data delivered by such computations. Quite similar problems are encountered for Large-Eddy Simulations of turbulent flames (Tabor et al., 1999) or for experimental investigations of flame/vortex interactions (Hargrave and Jarvis, 2006).

When considering quantitative problems like predictions of intermediate radicals, pollutant emissions, or ignition/extinction limits, the reaction processes should normally be described using complete chemical models (Hilbert et al., 2004). In the past, such computations relying on detailed models have been limited to two dimensions due to the huge numerical cost associated with three-dimensional DNS. But, of course, turbulence is fundamentally a three-dimensional process, so that two-dimensional simulations necessarily have a questionable validity and generality. This explains why several research groups are now focusing their efforts on three-dimensional DNS including a realistic description of the chemical reactions, as shown here.

The presented results illustrate our recent progress to carry out three-dimensional direct simulations of turbulent reacting flows. Two different DNS codes are employed to investigate different issues and flame configurations, involving different fuels. The code π^3 is a three-dimensional DNS code relying on a low-Mach number approximation to describe the turbulent flow. Chemical processes are computed thanks to a tabulation procedure, presented in details in other publications. For the case considered here (methane/air combustion) the tabulation employs two coordinates to enter a look-up table constructed with a complete reaction scheme, containing 29 species and 141 individual reactions.

The second code, *Sider* is an explicit three-dimensional DNS code solving the fully compressible reactive Navier-Stokes equations. In this code the chemical processes are directly computed using a complete reaction scheme and accurate transport properties are taken into account to describe molecular diffusion. It has been used in the present work to investigate the structure of a hydrogen/air turbulent non-premixed flame. The corresponding complete reaction scheme considers 9 chemical species and 38 chemical reactions.

Comparing both DNS codes, it is clear that *Sider* contains more accurate physical models and is able to treat problems (for example flame/acoustic interactions) not directly accessible with π^3. But this is associated with a computing cost 10 to 100 times higher than the corresponding computing time requested by π^3. Both codes are therefore perfectly complementary. When a high accuracy is required, *Sider* must be employed, but with a corresponding, very long computing time. For more systematic studies requesting several computations, π^3 is the only viable alternative.

Case 1, computed with π^3, corresponds to the growth of a spherical flame kernel in a turbulent flow. The flame is initially perfectly spherical, laminar and centered in the middle of the numerical domain. A field of synthetic homogeneous isotropic turbulence is superposed on top of this laminar configuration. The coupled process is then computed using the low-Mach number approximation for the flow. As a result, a turbulent, fully premixed flame expands into the numerical domain.

Case 2, computed with *Sider*, corresponds to the time-dependent evolution of a turbulent non-premixed flame between a diluted fuel and an oxidizer. The initial configuration is a perfectly planar, laminar flame. Again, a field of synthetic homogeneous isotropic turbulence is generated and superposed on top of this laminar configuration. The coupled problem is then computed further using the fully compressible Navier-Stokes equations. As a result, a turbulent, non-premixed flame develops into the numerical domain.

2. Mathematical and Physical Models

2.1 DNS Code π^3

This three-dimensional DNS code has been developed using Fortran 95. A strong reduction of the needed computing times is obtained by combining a low-Mach number approach, well suited to most practical configurations involving combustion, with an accurate reduction technique for the chemistry, called FPI. This code and reduction method have been already described in previous publications (e.g. Thévenin et al., 2002). The code π^3 thus does not rely on complete reaction schemes to describe the chemistry. This is of course the most accurate technique (see next section) but rapidly leads to unacceptable computing costs in three dimensions (Hilbert et al., 2004). As an alternative to complete reaction schemes, a method called FPI has been developed (Gicquel et al., 2000), leading to a tabulation of the chemical reaction terms into a look-up table before the DNS computation (Fiorina et al., 2003). For most cases, flame speed, extinction limits and radical profiles are predicted almost exactly using FPI when compared to the complete reaction scheme. The FPI database used in the present computations is the same as previously employed in Thévenin et al. (2002) and is obtained using the complete reaction scheme of Lindstedt (1998) including 29 species and 141 reactions to describe methane/air combustion. The look-up table is simply parameterized by two coordinates and has been computed using a unity Lewis number hypothesis for the sake of simplicity. For the conditions retained for Case 1, the laminar flame speed obtained using multi-component diffusion velocities is almost identical to that computed with a simple unity Lewis number hypothesis (relative error below 5 %), showing that in this case such a simplification should be acceptable.

For the flow equations, a low-Mach number formulation based on a projection method is retained to further speed-up the DNS computations. Due to this fact, acoustic waves are automatically removed from the solution. It is therefore not clear at first if this approach could lead to valid results for turbulent combustion. To explore this point, a detailed validation procedure has been carried out (de Charentenay et al., 2002). It has been possible to demonstrate that the error implied by the low-Mach number approximation is negligible when investigating the turbulent flame structure and its evolution.

Combining the low-Mach number approach and the chemistry reduction using FPI leads to a typical speed-up of one or two orders of magnitude compared to a fully compressible formulation employing complete reaction schemes, like *Sider*. Thanks to this considerable acceleration, three-dimensional DNS at moderate Reynolds numbers become feasible on a small PC cluster or even on a single, standard PC. For example, three-dimensional results of Case 1 presented here have been computed on a single Pentium 2.6 GHz PC with 2 GB of memory. Typical computing times are about 100 hours per computation.

2.2 DNS Code Sider

For a more accurate description of all physical processes including acoustics, Direct Numerical Simulations of reactive flows are carried out by solving the compressible multi-species Navier-Stokes equations (Kuo, 1986).

Sider is a recent, three-dimensional extension of the older, two-dimensional code *parcomb* developed by Thévenin and co-workers (Thévenin et al., 1996). It is a Fortran 95, finite-difference DNS code solving the compressible Navier-Stokes equations for multicomponent reacting flows. Derivatives are computed using sixth-order central approximations within the numerical domain. A fourth-order four-stage Runge-Kutta algorithm realizes the temporal integration. The adaptive timestep is controlled by three independent mechanisms. A Courant-Friedrichs-Levy (CFL) condition and a Fourier condition (for the diffusion terms) are tested in order to ensure the stability of the explicit integration. Using timestep doubling, the size of the timestep is also limited by a condition based on the accuracy of the result (Press et al., 1989). Boundary conditions are formulated using the Navier-Stokes Characteristic Boundary Condition (NSCBC) technique (Poinsot and Lele, 1992), extended to take into account multicomponent thermodynamic properties (Baum et al., 1994).

Transport coefficients and chemical kinetics are treated in a similar way to the methods implemented in the standard packages CHEMKIN II and TRANSPORT (Kee et al., 1980, 1983). To compute the chemical reactions, *Sider* fully considers the influence of all chemical species and reactions, based on a complete reaction scheme (Warnatz et al., 2001). The influence of each reaction is computed thanks to an Arrhenius law. This exact description is of course much more accurate but leads to considerably longer computing times compared to the tabulated chemistry implemented in π^3.

The DNS code *Sider* has been both vectorized and parallelized and is now used extensively to investigate turbulent flames.

3. Numerical Configurations and Problem Parameters

Case 1, computed with π^3, corresponds to the expansion of a flame kernel in a turbulent flow. The flame is initially perfectly spherical, laminar and centered in the middle of the numerical domain. A field of synthetic homogeneous isotropic turbulence is then superposed on top of this laminar configuration. The coupled process is finally computed using the low-Mach number approximation for the flow. As a result, a turbulent, fully premixed flame expands into the numerical domain. Initial turbulence properties are checked by a post-processing. To illustrate the procedure, this leads for example in Case 1 to a Reynolds number $\mathrm{Re}_{l_t} = 167$ with an integral scale of turbulence $l_t = 1.88$ mm, a turbulent fluctuation velocity $u' = 1.56$ m/s and a value of the unburnt mixture viscosity $\nu = 1.76 \times 10^{-5}$ m^2/s. The characteristic time-scale of the large turbulent structures is then $\tau_{l_t} = 1.2$ ms. In all simulations the grid spacing is constant and uniform, equal for example to 55 μm in Case 1. Each side of the computational domain is 6.5 mm long, leading to a computational grid with roughly 1.7 million grid points. A fully premixed methane/air flame at an equivalence ratio $\phi = 1.59$ (rich flame), atmospheric pressure and fresh gas temperature of 300 K is considered in the computation.

For Case 2, where a three-dimensional non-premixed flame between diluted hydrogen and air develops within a turbulent flow, the computational domain is a cube of 1 cm side. Along each direction, 200 points are regularly spaced, leading to 8 million grid points. The fuel (diluted H_2) occupies initially half of the computational domain, the oxidizer the other half. Hydrogen is diluted with nitrogen in order to obtain a global mixture ratio of 0.8. The initial temperature is 298 K everywhere; ignition is obtained at the contact interface between fuel and oxidizer by temporary heat addition. The characteristic time-scale of the large turbulent structures is here $\tau_{l_t} = 0.75$ ms. For both cases, the time-dependent DNS is continued during a time at least equal to τ_{l_t}, in order to obtain flame/turbulence equilibrium (Rutland et al., 1990).

4. Results and Discussions

4.1 Case 1: Expansion of a Turbulent Premixed Flame

The time-evolution of the expanding turbulent premixed flame is shown in Fig. 1. The flame position is defined as the isosurface of the mass fraction $Y(CO_2) = 0.03$, since this value corresponds to the steepest temperature gradient in the associated one-dimensional laminar premixed flame. The strong impact of turbulence on the development of the initially spherical flame is clearly observed in this figure through the large wrinkling and deformation of the initial flame. Furthermore, many important modeling quantities are extracted from the results. This post-processing delivers in particular locally strain-rate, flame curvature and flame thickness. In Fig. 1 the flame surface is for example colored by the instantaneous local strain rate. Furthermore, the normalized distribution of curvature along the flame front at $t = 1.2$ ms has been determined. The flame front is extracted from the data, its normal vector is computed and flame front curvature is given by its divergence. This procedure has been automated using the commercial packages Tecplot and Matlab. As a complement, the normalized distribution of flame thickness at $t = 1.2$ ms has been also computed. We rely on the temperature gradient along our flame, leading to a thermal flame thickness $\delta = (T_b - T_u)/(\partial T / \partial x)$. Figure 2 depicts the local flame curvature (left) and local flame thickness (right) on top of the flame surface. From these pictures a non-negligible correlation between curvature and thickness is already visible, which should be considered in corresponding models.

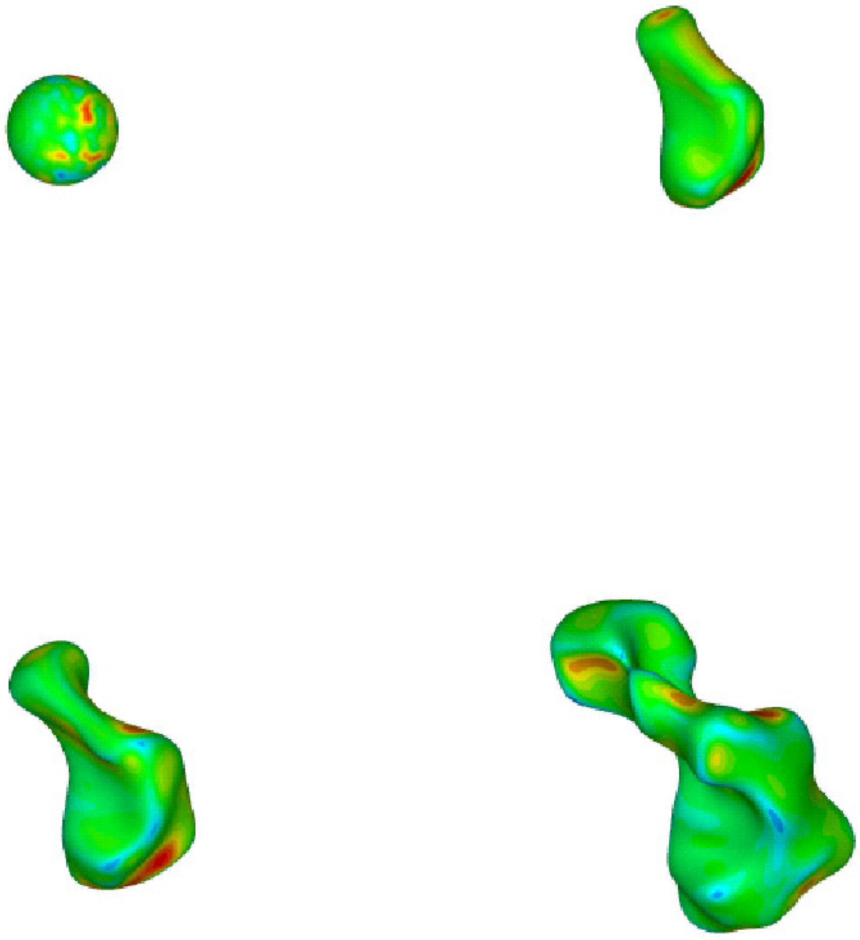

Fig. 1. Successive positions of the flame front, colored with tangential strain-rate value. Four solutions are shown, corresponding respectively to a time $t = 0$, 0.4, 0.6, 1.0 ms (from left to right and top to bottom). Case 1 is associated with an integral scale of turbulence $l_t = 1.88$ mm and a grid resolution of 55 μm.

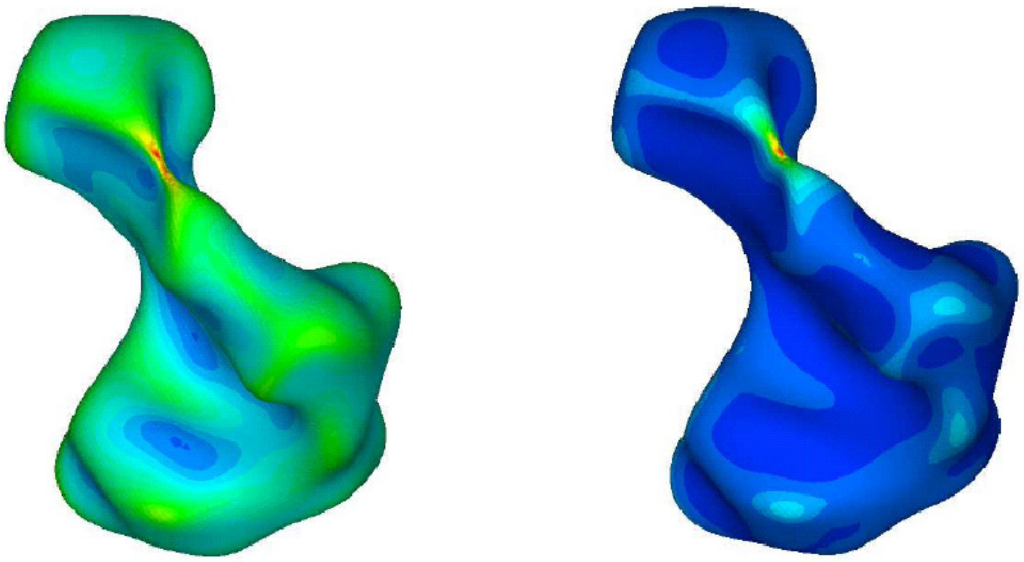

Fig. 2. Instantaneous flame front at t = 1.0 ms, colored with local mean flame curvature (left) or local flame thickness (right). Case 1 is associated with an integral scale of turbulence $l_t = 1.88$ mm and a grid resolution of 55 µm.

4.2 Case 2: Structure of a Turbulent Non-Premixed Flame

The time-dependent evolution of a non-premixed flame interacting with turbulence is computed in Case 2. Periodicity is assumed in the y and z-directions, while both x-boundaries are handled using non-reflecting boundary conditions. An example of the corresponding results is presented in Fig. 3 and 4, where the temperature and heat release of the flow field are shown at t = 1.0 ms. Regions showing a very strong increase of the local heat release can be observed as well as regions where the flame is locally extinguished.

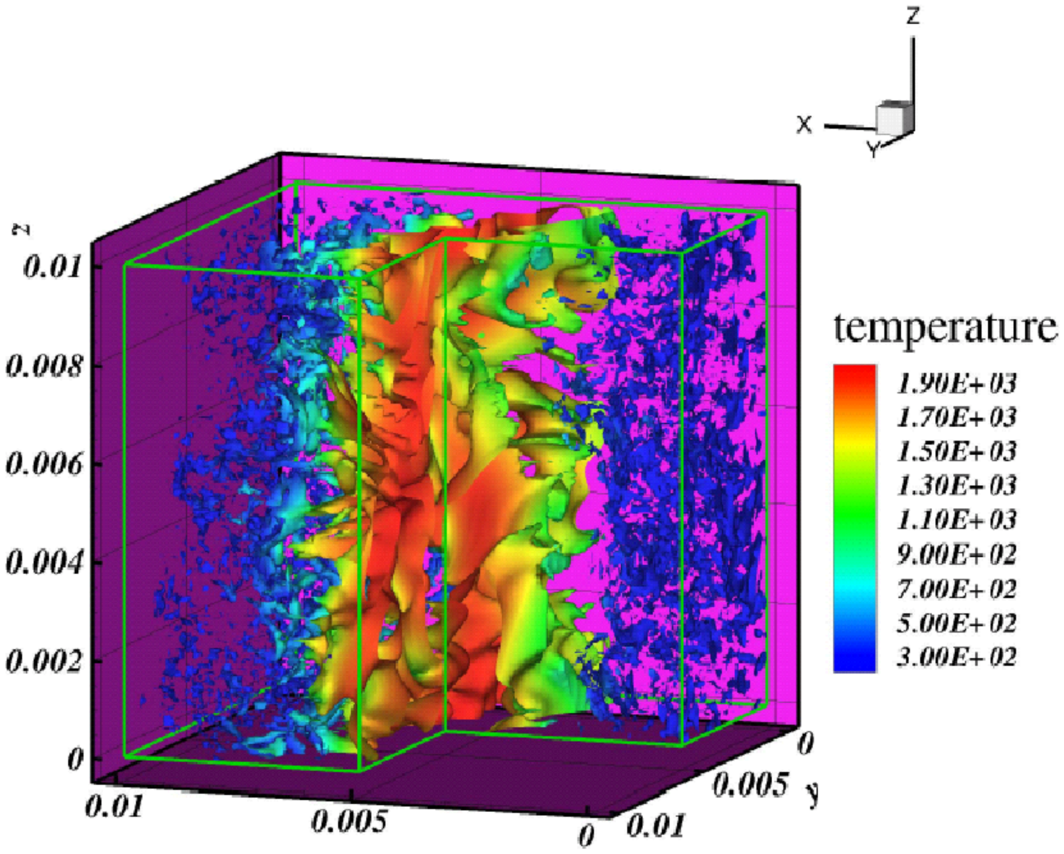

Fig. 3. Temperature in a turbulent H_2/air non-premixed flame at t = 1.0 ms.

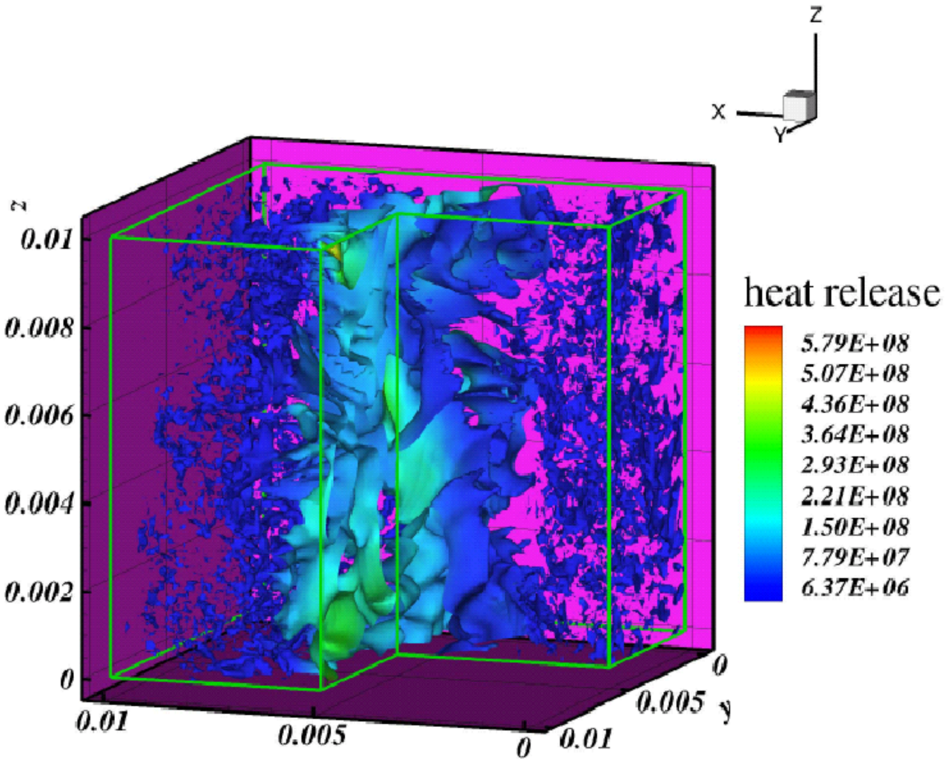

Fig. 4. Heat release in a turbulent H_2/air non-premixed flame at t = 1.0 ms.

To define a non-premixed flame front, a mixture fraction Z is classically computed based on the element mass fractions of hydrogen and oxygen (Hilbert et al., 2004). The value of Z corresponding to local stoichiometric conditions is highlighted in green color in Fig 5. Furthermore, the limits of the mixing region (Z = 0.1, blue, and Z = 0.9, orange) are also presented. An isosurface of heat release corresponding to 90 % of its peak value is finally represented with a purple color in this figure. It can be clearly observed that maximum heat release is concentrated in the vicinity of the stoichiometric conditions for this case. The very complex instantaneous structure of the turbulent flame is also obvious from this figure.

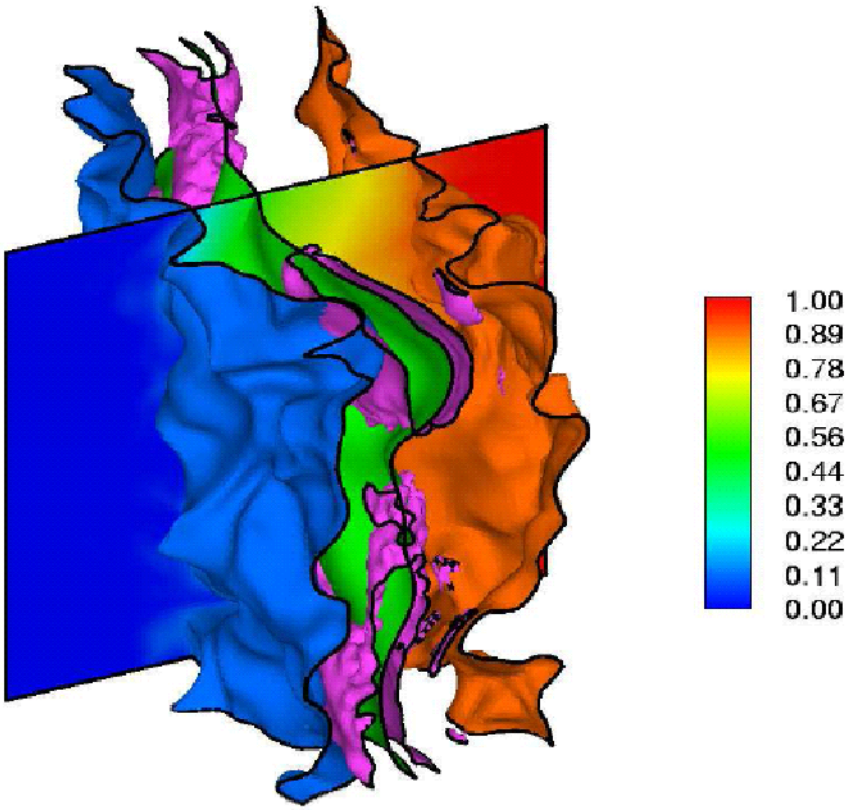

Fig. 5. Instantaneous flame front at t = 1.0 ms, showing stoichiometric conditions (green), mixing region limits (blue: oxidizer side; orange: fuel side), and instantaneous heat release isosurface (purple).

5. Conclusions

In this paper results obtained with Direct Numerical Simulations have been presented. Different turbulent flames corresponding to two different combustion regimes (premixed, Case 1; non-premixed, Case 2) and fuels (methane, Case 1; hydrogen, Case 2) have been computed using DNS and post-processed in order to extract important quantities. Thanks to such results, it is possible to improve our understanding of the complex coupling processes occurring in such configurations. Furthermore, existing simplified models employed to describe turbulent combustion can be checked, validated, improved or revised by comparison with DNS results, considered as a reference information. At present, a systematic post-processing toolbox is being written to facilitate as far as possible a detailed analysis of the wealth of raw data delivered by DNS.

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