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Highly resolved numerical simulation of combustion in supersonic hydrogen–air coflowing jets

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ABSTRACT

The present study is focused on the analysis of non-premixed combustion in high-velocity (supersonic) flows. The computations make use of a large eddy simulation (LES) model, which has been recently introduced to address combustion in high Reynolds number turbulent flows featuring moderate Damköhler values. We expect that the corresponding closure is able to account for the specificities encountered in high Mach number turbulent reactive flows featuring chemical reaction time scales with the same order of magnitude as flow time scales. The model takes finite-rate chemistry and micro-mixing effects into account within the framework of the partially stirred reactor (PaSR) concept, it is hereafter denoted by U-PaSR (*unsteady partially stirred reactor*). (i) In a first step of the present investigation, the capabilities of the U-PaSR closure hence proposed are evaluated through a detailed comparison performed between numerical results and the data obtained from an experimental study devoted to non-premixed combustion in supersonic co-flowing jets of hydrogen and vitiated air. The simulated test case corresponds to a well-documented experimental database that includes Raman scattering and laser-induced pre-dissociative fluorescence measurements. The comparisons performed between computational results and experimental data establish that the physical processes are well-described by the performed simulation. (ii) In a second step of this study, the flame structure and associated stabilization zone are analysed in the light of numerical simulation results. The post-processing to the computational results indeed confirms the importance of self-ignition processes, as well as the relevance of diagnostic tools recently introduced by Boivin et al. [1,2]. Considering the stabilization zone, it also emphasizes the essential importance of the pressure dynamics associated with the discharge of compressible coflowing jets into the atmosphere – an importance that was not so clearly evidenced from previous numerical simulations conducted on the same experimental benchmark.

1. Introduction

The scramjet (supersonic combustion ramjet) engine is conceptually a ramjet in which the compressed air flow from the inlet is kept supersonic throughout the whole flowpath. These engines are designed for airbreathing propulsion of vehicles at high Mach number values (above 5 or 6) where practical ramjet engines feature lower performance, especially in term of specific impulse [3–5]. The corresponding conditions concern several fields of application including civil transport, space launchers or missiles.

In comparison with experimental investigations, which remain very challenging to conduct in such flow conditions, computational fluid dynamics (CFD) offers an attractive alternative and nonetheless complementary tool for the study of such high-speed turbulent reactive flows. However, the most standard and efficient closures, which are based on the fast chemistry approximation, become less appropriate for such type of conditions, which are governed by finite-rate chemistry effects and ignition phenomena. In the corresponding conditions, chemical reaction time scales tend indeed to be the same order of magnitude as turbulent time scales, with resulting Damköhler number values close to unity. In such regimes of combustion, the application of fast chemistry assumptions associated with either equilibrium approximation or flamelet closures, where the flow field modeling is decoupled from chemistry, therefore becomes less appropriate, and finite-rate chemistry-based closures seem therefore more appealing to describe supersonic combustion, which is dominated by chemical processes including self-ignition phenomena.

The focus of the present study is thus placed on the application of such a closure proposal to supersonic turbulent combustion. The unsteady partially stirred reactor (U-PaSR) closure is presently

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used to account for the inhomogeneities of both composition and temperature inside the flame region. The retained experimental benchmark is a well-documented configuration that consists of a supersonic lifted co-flowing hydrogen–air non-premixed jet flame. The objective with the present manuscript is twofold. The first target is to assess the U-PaSR closure against a well-documented database. The second intent is associated with the analysis of the stabilization zone. In contrast with the recent study of Boivin et al. [2], it is found that there are two essential but distinct regions in the flowfield, one near the exit, which is related to the formation of hydroperoxyl (HO_2) radicals, and one further downstream, related to shock compression, associated temperature rise and subsequent heat release.

The present manuscript is organized as follows: the next section is devoted to the presentation of the numerical model. It is followed by the description of the supersonic lifted flame with emphasis not only placed on experimental investigations that were conducted but also on numerical studies previously devoted to the same benchmark. Finally, after a brief presentation of the numerical setup, including mesh and boundary conditions, the last section gathers computational results. A detailed comparison between computations and available experimental data is provided, it is supplemented with a comparison performed with previous numerical results obtained on the same experimental benchmark. Finally, the obtained results are subsequently used to analyse the non-premixed flame structure and stabilization processes.

2. Numerical model

2.1. Mathematical model

The set of governing equations corresponds to the compressible conservative form of the reactive Navier–Stokes equations. It includes balance equations for mass, mass fractions of chemical species, momentum and energy and describes convection, diffusion and chemical reactions [6]. We assume Fourier heat conduction and Fickian diffusion for the molecular contributions. Soret and Dufour effects, body forces as well as heat transport by radiation are neglected. The classical Reynolds averaging is not well-suited to compressible flows since it introduces many additional unknown correlations associated with density fluctuations. A mass-weighted Favre averaging is therefore preferred, so that the mean value of any quantity Φ is defined by $\widetilde{\Phi} = \overline{\rho\Phi}/\overline{\rho}$, where the overbar denotes the classical averaging (or filtering) procedure and with ρ the density of the mixture.

The subgrid scale (SGS) stress tensor $\overline{\rho}T_{ij} = \overline{\rho u_i u_j} - \overline{\rho}\widetilde{u}_i\widetilde{u}_j$ is modeled using the Boussinesq approximation $(T_{ij} - \delta_{ij}T_{kk}/3) = -2\nu_{SGS}(\widetilde{S}_{ij} - \delta_{ij}\widetilde{S}_{kk}/3)$ with the SGS viscosity obtained from $\nu_{SGS} = (C_s\Delta)^2 \mid \widetilde{S} \mid = (C_s\Delta)^2(2\widetilde{S}_{ij}\widetilde{S}_{ij})^{1/2}$ where $\widetilde{S}_{ij} = (\partial\widetilde{u}_i/\partial x_j + \partial\widetilde{u}_j/\partial x_i)/2$ is the strain rate tensor associated with the resolved velocity field $\widetilde{u}_i$ and C_s denotes the Smagorinsky constant. The isotropic contribution T_{kk}, corresponding to twice the subgrid scale turbulent kinetic energy, remains unknown. This term is usually neglected but it can also be modeled, for instance by using the Yoshizawa's expression [7]. The former solution is retained here for the sake of simplicity. Finally, the SGS scalar flux components are represented within the gradient law approximation with the SGS diffusivity evaluated from $(C_s\Delta)^2 \mid \widetilde{S} \mid /Sc_{SGS}$ with Sc_{SGS} a subgrid scale turbulent Schmidt number set to 0.7.

2.2. Turbulence–chemistry interaction (TCI) model

The high non-linearity (Arrhenius Law) of the instantaneous reaction rate $\dot{\omega}_k(T, Y_k)$ makes its filtered or averaged counterpart very difficult to model. When dealing with high-speed (supersonic) combustion applications, a first-order simplification is often retained as a preliminary step within the framework of the quasi-laminar (QL) combustion assumption, or homogeneous reactor (HR) approximation, that ignores the influence of composition and temperature fluctuations, i.e. the SGS chemical rate of any species k is approximated with $\dot{\omega}_k(\widetilde{T}, \widetilde{Y}_k)$. However, the composition fluctuations may play a crucial role in the processes of thermal runaway that take place in the mixing layer until ignition occurs. The unsteady partially stirred reactor (U-PaSR) concept thus offers an interesting basis to incorporate the effects associated to these inhomogeneities within either a Reynolds-averaged Navier–Stokes (RANS) or a large eddy simulation (LES) framework. Since the U-PaSR closure shares the same basis as the eddy dissipation concept (EDC) model introduced in the early works of Vulis [8], and Magnussen, see references [9–11], we first briefly summarize below the salient features of the EDC closure.

2.2.1. The EDC model

The EDC closure introduced by Magnussen relies on the highly intermittent character of the turbulence and implies that chemical reactions occur in fine-scale structures where most of the viscous dissipation and molecular mixing processes take place. Scalar dissipation indeed tends to form fine and elongated structures in space. As far as non-reactive scalars are considered, it is also remarkable that scalar gradient fluctuations are preferentially aligned with the direction of most compressive strain rate. In fact, experimental as well as numerical investigations have revealed that the scalar gradient field is more intermittent than the velocity gradient field [12]: the scalar dissipation rate (SDR) is indeed more intermittent than the turbulence dissipation rate. Turbulent mixing operates in the vicinity of very fine scale elongated structures, i.e. filament-like vortex structures or *worms*, the transverse dimension of which are of the order of the Kolmogorov length scale η_K (between 6 and 10 η_K). The scientific literature describes these regions of strong dissipation as sheet-like structures that surround the high enstrophy swirling *worms*. The reader may refer to [13,14] for further insights in the implications of recent progresses made in the description of small scale turbulence on turbulent combustion modeling. In non-premixed conditions, such as those considered therein, the nature of turbulent scalar mixing (i.e. SDR) is thus very intermittent and the closures discussed below are based on this intermittent nature of large Reynolds number turbulence. The structures that concentrate dissipation (mixing) processes (herein associated to the state *) coexist with non-homogeneous but weak vorticity zones (state 0), often referred to as a structureless *random sea*, where scalar mixing is simply considered as inefficient.[1] In the EDC model, each elementary volume of fluid is thus divided into fine-scale structure regions (denoted by *) featuring high scalar dissipation rates levels, and surroundings (denoted by ^{0}). The fine-scale structure regions (*) are supposed to behave like well-stirred reactors, i.e. perfectly stirred reactor (PSR), with potentially high reaction rates due to favorable mixing conditions, and surrounded by other regions (0) featuring vanishingly small reaction rate. From a general point of view, the mean reaction rate $\overline{\dot{\omega}}_k$ can be expressed as:

$$\overline{\dot{\omega}}_k = \int_{\Psi} \mathcal{P}(\psi)\dot{\omega}_k(\psi)\,d\psi \tag{1}$$

where $\mathcal{P}$ denotes the joint scalar PDF (Probability Density Function), $\psi = [T, Y_k]^T$ is the sample composition vector and Ψ is the associated domain of definition of the PDF. Considering the important levels of mixing rate in zone (*), it is supposed to behave as a homogeneous

[1] It should be acknowledged that the regions of weaker enstrophy may be less dynamically unimportant in turbulence than was previously thought.