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Highly-resolved large-eddy simulations of combustion stabilization in a scramjet engine model with cavity flameholder

Fábio Henrique Eugênio Ribeiro^{a,b}, Radouan Boukharfane^{a,c}, Arnaud Mura^{a,*}

^a*Institut Pprime UPR 3346 CNRS, ISAE ENSMA and University of Poitiers, France*

^b*Instituto de Estudos Avançados, São José dos Campos, SP, Brasil*

^c*Extreme Computing Research Center (ECRC), Computer Electrical and Mathematical Science and Engineering Division (CEMSE), KAUST, Thuwal, Saudi Arabia*

Abstract

Scramjet engines are high-speed airbreathing propulsion systems that do not require rotating elements to compress the air inlet stream. It is compressed dynamically through a supersonic intake system that is integrated in the forebody, thus leading to the required temperature and pressure levels for combustion to proceed within the combustor length. In such engines, the combustion chamber is crossed by a supersonic flow, which limits the time available to inject fuel, to mix it with oxidizer, to ignite the resulting mixture, and to reach complete combustion. Residence times can be increased thanks to cavities, which have the potential to stabilize combustion without excessive total pressure loss and are therefore used as flameholders in supersonic combustors. In the present study, we perform high-fidelity large-eddy simulations (LES) of a hydrogen jet in a supersonic crossflow (JISCF) of vitiated air, which is located upstream of a wall-mounted squared cavity. The performance of such high-fidelity LES does not only require the use of high-precision numerical schemes and reliable subgrid-scale models relevant to the so-called direct numerical simulation (DNS) limit, it is also strongly dependent on the mesh quality. Therefore, the present study places special emphasis on computational grid assessment through the introduction of a detailed numerical procedure, which aims at analysing mesh reliability. The corresponding procedure combines several verification subsets including (i) the inspection of distributions of the dimensions of the computational cells present at the wall location, (ii) the analysis of normalized velocity profiles and viscosity ratio in boundary layers, and (iii) the check of fields of some mesh quality indexes and associated distributions. For the geometry under consideration, it appears that the level of resolution imposed by a correct description of boundary layers leads to a mesh quality that is close to the one associated to DNS requirements. Combustion stabilization is then studied for two distinct values of the inlet vitiated airstream temperature. Two stabilization modes are recovered from the numerical simulations: cavity-stabilized and jet-wake stabilized regimes.

Keywords: High-speed flows, Large-eddy simulation (LES), Mesh reliability, Jet in supersonic crossflow (JISCF), Scramjet, Immersed boundary method (IBM)

*Corresponding author

Email address: `arnaud.mura@ensma.fr` (Arnaud Mura)

1. Introduction

Scramjet engine is a very promising propulsion strategy for hypersonic vehicles. Several fields of application, such as civil transport and launchers, are concerned. For access-to-space applications in particular, the use of airbreathing hypersonic propulsion systems could reduce significantly the launch costs. Preliminary studies showed remarkable and promising results in the use of this technology as a second stage of a three-stage-to-orbit launcher (Smart and Tetlow, 2009). Thus, there is a special interest in the hypersonic vehicle as the promise of an airbreathing reusable system able to lift payloads into Earth orbit.

One of the main advantages of scramjets over concurrent technologies is related to the fact that it does not carry oxidizer, which is scooped directly from the atmosphere, thus providing a considerable weight reduction and allowing for higher payloads and specific impulses compared to standard rocket engines (Heiser and Pratt, 1994; Smart, 2008; Segal, 2009). This also means reduced costs, reduced complexity, and also lighter ground support. However, high-speed flights in the atmosphere raise several specific issues related, among others, to aerodynamic heating and vehicle drag, which impose the cooling of both the vehicle and the engine for prolonged operations. The corresponding high temperature levels also contribute to the dissociation of molecules, e.g. oxygen and nitrogen molecules decompose and recombine, and they may even ionize at higher speeds (Anderson, 1989; Segal, 2009). Since it produces no thrust at zero flight speed, such an engine must be ignited after it has been accelerated to its takeover speed thanks to a secondary propulsion system. The issues associated to ignition and propulsion efficiency during this takeover stage are thus important in the scramjet development but they lie outside the scope of the present study, which is concerned with combustion stabilization, once significant flight Mach number values are reached.

As emphasized above, there are several possible applications of scramjet engines, including civil high-speed aircrafts, space exploration as reusable stages for access to Earth orbit, and military hypersonic weapons (Urzay, 2018). Despite many impressive achievements obtained in the field since the early sixties, still today there are no scramjet engines being used in practical devices: many developments including experimental flights and ground-based testings are currently in progress. In such engines, the combustion chamber is crossed by a supersonic flow, which limits considerably the time available to inject fuel, mix it with the oxidizer, ignite the resulting mixture, and stabilize combustion. Combustion ignition and stabilization indeed appears as one of the most challenging issues (Cai et al., 2018). One promising solution is the wall-mounted cavity, which has been shown to be quite efficient in stabilizing combustion without excessive total pressure loss (Ben-Yakar and Hanson, 2001; Mathur et al., 2001; Gruber et al., 2004). The recirculation zones that develop inside the cavity increase the residence time of intermediate combustion products that can continuously initiate chemical reactions. However, the understanding of the interaction of the fuel jet with the wall-mounted cavity is far from being an easy task (Cai et al., 2016; Gong et al., 2017) and it has motivated a large amount of experimental studies in both reactive and non-reactive conditions. For instance, Ben-Yakar and Hanson (2001) investigated hydrogen normal injection in air cross-flow upstream of a cavity simulating Mach 10 flight conditions. High-speed Schlieren visualization

42 and planar laser-induced fluorescence (OH-PLIF) were used to characterize the compressible
43 flow topology and combustion development. The first OH fluorescence events are found to take
44 place in the recirculation zone upstream of the underexpanded jet and the signal of fluores-
45 cence extends further downstream along the outer edge of the jet. Micka and Driscoll (2008)
46 studied the combustion characteristics of a dual-mode scramjet combustor with normal fuel
47 injection upstream of a cavity flame-holder. Depending on the value of the vitiated airstream
48 stagnation temperature, combustion is either anchored at the cavity leading edge and spreads
49 into the main flow at an approximately constant angle (low stagnation temperature levels)
50 or stabilizes a short distance downstream of the hydrogen injection, in its wake, and features
51 a curved leading edge (high stagnation temperature levels). The combustion stabilization is
52 analysed on the basis of premixed flame propagation and the possibility that it flashes for-
53 ward to a relatively stable location in the hydrogen jet-wake. Sun et al. (2008) also analysed
54 combustion in a supersonic combustor with normal hydrogen injection upstream of cavity
55 flame-holders. Their investigation is based on the combination of experimental observations
56 using OH-PLIF and numerical simulations performed within a hybrid RANS/LES framework.
57 It is shown that an approximately steady flame may be maintained in the cavity shear layer.
58 Hot combustion products can be transported towards the jet inlet stream through a process
59 of interaction between the counter-rotating vortices issued from the jet and the cavity shear
60 layer.

61 In the present study, it is attempted to perform high-fidelity numerical simulations of
62 a scramjet model representative of experimental investigations previously conducted at the
63 University of Michigan (Micka and Driscoll, 2009; Micka, 2010). In the experiments un-
64 der consideration, a sonic jet of hydrogen is injected into a supersonic crossflow of vitiated
65 air upstream of a wall-mounted cavity. The computations are performed with the high-
66 performance computational solver **CREAMS** (Martínez-Ferrer et al., 2014, 2017a) that has been
67 developed to perform the numerical simulation of compressible reactive multi-component flows
68 on massively-parallel architectures. The solver makes use of high-order precision numerical
69 schemes applied on structured meshes. The simplified computational geometry consists of
70 a constant section channel, followed by the wall-mounted cavity section, and finally the di-
71 verging section. This geometry is handled thanks to the recent immersed boundary method
72 (IBM) introduced by Boukharfane et al. (2018). The corresponding set of computations is
73 expected to be useful to analyse the reactive flow topology and structure as well as combustion
74 regimes, which can be investigated on the basis of standard turbulent combustion diagrams.
75 Combustion stabilization is studied for two distinct values of the inlet vitiated air-stream
76 temperature, which are denoted RFSC-LST and RFSC-HST, for low- and high-stagnation
77 temperature levels, respectively. A preliminary inspection of numerical data confirms that
78 two stabilization modes can be observed: cavity stabilization mode for case RFSC-LST and
79 jet-wake stabilization mode for case RFSC-HST.

80 The present manuscript is organized as follows, in section 2, the large-eddy simulation
81 model and numerical methods are presented. It is followed by a short section where the
82 computational setup is set forth. This section includes the presentation of the computa-

83 tional domain, its discretization, and associated boundary conditions. The next part of the
 84 manuscript, section 4, provides a detailed analysis of computational resolution issues. Finally,
 85 some results of both non-reactive and reactive flow simulations are discussed in section 5. The
 86 manuscript ends with a brief conclusion section 6, where some perspectives for future works
 87 are also presented.

88 2. Governing equations and numerical methods

89 The present study is conducted within the large-eddy simulation (LES) framework, i.e., the
 90 largest scales of the flow are explicitly computed, while the subgrid-scale (SGS) effects, re-
 91 sulting from the smallest ones, are modelled. Thus, the following set of filtered transport
 92 equations, written in a conservative form, is used to describe the multicomponent reactive
 93 flowfield

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial \bar{\rho} \tilde{u}_j}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_i} = -\frac{\partial \bar{p}}{\partial x_j} + \frac{\partial \bar{\tau}_{ij}}{\partial x_i} - \frac{\partial}{\partial x_i} (\overline{\rho u_i u_j} - \bar{\rho} \tilde{u}_i \tilde{u}_j) \quad (2)$$

$$\frac{\partial \bar{\rho} \tilde{e}_t}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{e}_t}{\partial x_i} = -\frac{\partial \bar{p} \tilde{u}_i}{\partial x_i} + \frac{\partial \tilde{u}_i \bar{\tau}_{ij}}{\partial x_j} - \frac{\partial \bar{\mathcal{J}}_i}{\partial x_i} - \frac{\partial}{\partial x_i} (\overline{(\rho e_t + p) u_i} - (\bar{\rho} \tilde{e}_t + \bar{p}) \tilde{u}_i) \quad (3)$$

$$\frac{\partial \bar{\rho} \tilde{Y}_\alpha}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{Y}_\alpha}{\partial x_i} = -\frac{\partial \bar{\rho} \tilde{Y}_\alpha \tilde{V}_{\alpha i}}{\partial x_i} - \frac{\partial}{\partial x_i} (\overline{\rho Y_\alpha u_i} - \bar{\rho} \tilde{Y}_\alpha \tilde{u}_i) + \bar{\rho} \tilde{\omega}_\alpha \quad (4)$$

97 where t denotes time, x_i is the Cartesian coordinate in direction i (with $i = 1, \dots, 3$), u_i is the
 98 velocity component in the same direction, ρ is the density, p is the pressure, $e_t = e + u_i u_i / 2$ is
 99 the total specific energy which is obtained as the sum of the kinetic energy and internal specific
 100 energy e , and finally Y_α is the mass fraction of chemical species α (with $\alpha = 1, \dots, \mathcal{N}_{\text{sp}}$). The
 101 integer \mathcal{N}_{sp} denotes the number of chemical species. In the above equations, $\bar{\Phi}$ is the filtered
 102 value of any quantity Φ , while $\tilde{\Phi}$ denotes its density-weighted or Favre filtered counterpart:
 103 $\tilde{\Phi} = \overline{\rho \Phi} / \bar{\rho}$. The thermodynamic variables are interrelated through the filtered pressure field
 104 $\bar{p} = \bar{\rho} \mathcal{R} \bar{T} / \bar{\mathcal{W}}$ with \mathcal{R} the universal gas constant, T the temperature, and $\bar{\mathcal{W}}^{-1} = \sum_{\alpha=1}^{\mathcal{N}_{\text{sp}}} \tilde{Y}_\alpha / \mathcal{W}_\alpha$
 105 the molar weight of the multicomponent mixture (\mathcal{W}_α being the molar weight of species α). In
 106 Eq. (4), the quantities $V_{\alpha i}$ and $\dot{\omega}_\alpha$ denote the diffusion velocity and chemical production rate
 107 of species α , respectively. The filtered stress tensor is evaluated from $\bar{\tau}_{ij} = 2\tilde{\mu}(\tilde{S}_{ij} - \tilde{S}_{kk}\delta_{ij}/3)$
 108 with $\tilde{S}_{ij} = (\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i) / 2$ denoting the resolved strain-rate tensor. It is noteworthy
 109 that the retained system of filtered equations is similar to the one previously considered
 110 by Ragab et al. (1992), Piomelli (1999), Kosovic et al. (2002), and Dubois et al. (2002).

111 For the present set of numerical simulations, standard modelling assumptions are re-
 112 tained. A mixture-average formulation is used to describe multicomponent molecular diffu-
 113 sion (Hirschfelder and Curtiss, 1949). Moreover, it is assumed that the filtered molecular
 114 diffusion fluxes and filtered heat flux can be deduced from their instantaneous expressions,

115 but applied to filtered quantities. The components of the filtered molecular diffusion flux of
 116 chemical species α are thus approximated from

$$\overline{\rho Y_\alpha V_{\alpha i}} = -\bar{\rho} \tilde{D}_\alpha^m \frac{\mathcal{W}_\alpha}{\mathcal{W}} \frac{\partial \tilde{X}_\alpha}{\partial x_i} + \bar{\rho} \tilde{Y}_\alpha \tilde{V}_i^c \quad (5)$$

117 where X_α denotes the molar fraction of species α and \tilde{D}_α^m is the matrix of the diffusion flux
 118 coefficients of the same chemical species. It is worth noting that the last term of Eq. (5) is
 119 a correction term used to enforce total mass conservation. Indeed, at each time step, each
 120 component of the correction velocity $\tilde{V}_i^c = \sum_{\beta=1}^{\mathcal{N}_{\text{sp}}} \tilde{D}_\beta^m (\mathcal{W}_\beta / \mathcal{W}) \partial \tilde{X}_\beta / \partial x_i$ is evaluated and added
 121 to the filtered velocity component \tilde{u}_i so as to enforce compatibility between the discrete forms
 122 of total mass and species mass fractions conservation equations.

123 The i -component of the filtered molecular heat flux is expressed as follows:

$$\bar{\mathcal{J}}_i = -\tilde{\lambda} \frac{\partial \tilde{T}}{\partial x_i} + \sum_{\alpha=1}^{\mathcal{N}_{\text{sp}}} \bar{\rho} \tilde{Y}_\alpha \tilde{V}_{\alpha i} \tilde{h}_\alpha \quad (6)$$

124 where $\tilde{\lambda}$ is the thermal conductivity of the multicomponent mixture as evaluated from the
 125 filtered composition.

126 The subgrid-scale (SGS) stress tensor $T_{ij} = \overline{\rho u_i u_j} - \bar{\rho} \tilde{u}_i \tilde{u}_j$ is modelled within the Boussi-
 127 nesq's framework. Its deviatoric part is thus evaluated from $T_{ij} - T_{kk} \delta_{ij} / 3 = -2\mu_{\text{SGS}} (\tilde{S}_{ij} -$
 128 $\tilde{S}_{kk} \delta_{ij} / 3)$, where $\mu_{\text{SGS}} = \bar{\rho} \nu_{\text{SGS}}$ is the SGS eddy viscosity and T_{kk} denotes the isotropic con-
 129 tribution. The closure of the SGS mass fluxes relies on the standard turbulent diffusivity
 130 assumption, which may be expressed in the following general form:

$$T_{\varphi, i} = \overline{\rho \varphi u_i} - \bar{\rho} \tilde{\varphi} \tilde{u}_i = \bar{\rho} (\overline{\varphi u_i} - \tilde{\varphi} \tilde{u}_i) = -\bar{\rho} D_{\text{SGS}} \frac{\partial \tilde{\varphi}}{\partial x_i} \quad (7)$$

131 where φ denotes any scalar quantity, $D_{\text{SGS}} = \nu_{\text{SGS}} / \text{Sc}_{\text{SGS}}$ is the turbulent diffusivity and Sc_{SGS}
 132 corresponds to the SGS turbulent Schmidt number, the value of which is set to 0.7. Finally,
 133 the last term of the filtered energy equation, see Eq. (3), may be rewritten as follows:

$$\overline{(\rho e_t + p) u_j} - (\bar{\rho} \tilde{e}_t + \bar{p}) \tilde{u}_j = \underbrace{\left[\overline{\rho c_p T u_j} - \bar{\rho} \tilde{c}_p \tilde{T} \tilde{u}_j \right]}_{\mathcal{Q}_j} + \underbrace{\left[\frac{1}{2} (\overline{\rho u_i u_i u_j} - \bar{\rho} \tilde{u}_i \tilde{u}_i \tilde{u}_j) \right]}_{\psi_{ij}} - \frac{1}{2} T_{ii} \tilde{u}_j \quad (8)$$

134 where $\mathcal{Q}_j = -\lambda_{\text{SGS}} \partial \tilde{T} / \partial x_j$ is nothing but the SGS heat flux also modelled using the gradient-
 135 diffusion approximation, with $\lambda_{\text{SGS}} = \mu_{\text{SGS}} \bar{c}_p / \text{Pr}_{\text{SGS}}$ the turbulent thermal conductivity and
 136 Pr_{SGS} the SGS turbulent Prandtl number. The value of Pr_{SGS} is set to 0.7. In Eq. (8), the
 137 quantity ψ_{ijk} denotes the triple velocity correlation tensor, which is closed by retaining the
 138 Daly and Harlow expression $\psi_{ijk} = C_{c3} \nu_{\text{SGS}} \partial T_{ij} / \partial x_k$ with $C_{c3} = 0.08$ (Daly and Harlow,
 139 1970). At this level, it must be precised that the SGS eddy viscosity μ_{SGS} is evaluated from
 140 the wall-adapting local eddy (WALE) model of Nicoud and Ducros (1999):

$$\mu_{\text{SGS}} = \bar{\rho} (C_w \Delta)^2 \frac{(S_{ij}^d S_{ij}^d)^{3/2}}{(\tilde{S}_{ij} \tilde{S}_{ij})^{5/2} + (S_{ij}^d S_{ij}^d)^{5/4}} \quad (9)$$

141 where $C_w = C_s \sqrt{10.6}$ is the WALE model constant, $\Delta = (\Delta x_1 \Delta x_2 \Delta x_3)^{1/3}$ is the characteristic
 142 mesh size, and S_{ij}^d is the traceless symmetric part of the square of the resolved velocity gradient
 143 tensor:

$$S_{ij}^d = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_l} \frac{\partial \tilde{u}_l}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_l} \frac{\partial \tilde{u}_l}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \tilde{u}_m}{\partial x_l} \frac{\partial \tilde{u}_l}{\partial x_m} \delta_{ij} \quad (10)$$

144 The following set of computations have been performed with C_s set to its standard value $C_s =$
 145 0.18. In this respect, it should be emphasized that the present closure of the filtered Navier-
 146 Stokes equations gathers the same modelling ingredients as those previously retained by Techer
 147 et al. (2018). Finally, the filtered chemical rates $\tilde{\omega}_\alpha$ that appear in the right-hand-side of the
 148 filtered species mass fraction transport equations are represented using either the perfectly
 149 stirred reactor (PSR) or the unsteady partially stirred reactor (U-PaSR) closure (Berglund
 150 et al., 2010; Moule et al., 2014a). These two SGS closures make use of a detailed description
 151 of chemistry and the mechanism of O’Conaire et al. (2004), consisting of 9 chemical species
 152 (H_2 , O_2 , H_2O , H , O , OH , HO_2 , H_2O_2 and N_2) and 21 elementary reaction steps, is used to
 153 represent H_2 -air chemistry. Additional details about these two SGS turbulent combustion
 154 closures will be provided in the next sections of the manuscript.

155 Computations are performed with the computational fluid dynamics (CFD) solver **CREAMS**.
 156 The reader is referred to Martínez-Ferrer et al. (2014) and to Boukharfane et al. (2018) for
 157 an exhaustive presentation of this solver including its application to a large number of verifi-
 158 cation test cases. Its main features are as follows: the treatment of the inviscid component of
 159 the transport equations relies on a seventh-order accurate weighted essentially non-oscillatory
 160 (WENO7) reconstruction of the characteristic fluxes. In practice, the numerical solver uses a
 161 high-order accuracy finite difference scheme, and the application of the nonlinear weighting
 162 procedure of the WENO7 scheme is conditioned to a shock sensor that involves the local values
 163 of the normalized spatial variations of both pressure and density (Buttay et al., 2016). The
 164 viscous and molecular diffusion fluxes are evaluated thanks to an eighth-order centered finite
 165 difference scheme. The temporal integration is performed using a third-order Runge-Kutta
 166 algorithm. Finally, the present set of computations makes use of a recent immersed bound-
 167 ary method (IBM) to describe the wall-mounted cavity. The corresponding IBM strategy
 168 combines direct-forcing (DF) and ghost-point-forcing (GPF) algorithms (Boukharfane et al.,
 169 2018).

170 3. Computational setup

171 Figure 1 displays the supersonic combustion facility studied at the University of Michigan.
 172 It consists of a two-dimensional Mach 2.2 nozzle, a constant area isolator that extends over
 173 400.0 mm up to the leading edge of a rectangular cavity, which is followed by a 349.0 mm
 174 long and 4 degree diverging section dumping into a 152.0 mm diameter exhaust. The cavity
 175 spans the entire width of the test section, which is equal to 38.1 mm. It is 50.8 mm long and
 176 12.7 mm high, thus featuring a rather small length to depth ratio ($l_2/h_2 \leq 10.0$) in such a
 177 manner that it can be considered as an open cavity (Lawson and Barakos, 2011). Upstream

178 of this wall-mounted cavity, a sonic hydrogen jet is injected into the vitiated air supersonic
 179 crossflow .

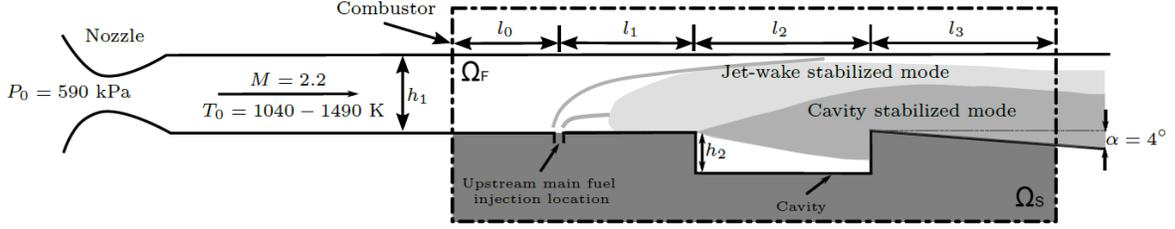


Figure 1: Schematics of the combustion facility with the computational domain highlighted

180 The computational domain, highlighted in Fig. 1, is restricted to the consideration of the
 181 transverse jet and cavity flowfield. It can be decomposed into three distinct parts: a constant
 182 section channel s_1 with length $L_{x_1,s_1} = l_0 + l_1 = 94.5$ mm and height $L_{x_2,s_1} = h_1 = 39.4$ mm,
 183 a section s_2 with length $L_{x_1,s_2} = l_2 = 50.8$ mm featuring the wall-mounted cavity with depth
 184 $h_2 = 12.7$ mm, and a four-degree diverging section s_3 with length $L_{x_1,s_3} = l_3 = 76.2$ mm. The
 185 total length of the computational domain is thus $L_{x_1} = 221.5$ mm and it is $L_{x_3} = 38.1$ mm
 186 in the spanwise direction. Section s_1 features the hydrogen injection port with diameter
 187 $D_1 = 2.5$ mm located along the combustor centerline at 44.5 mm upstream of the cavity
 188 leading edge.

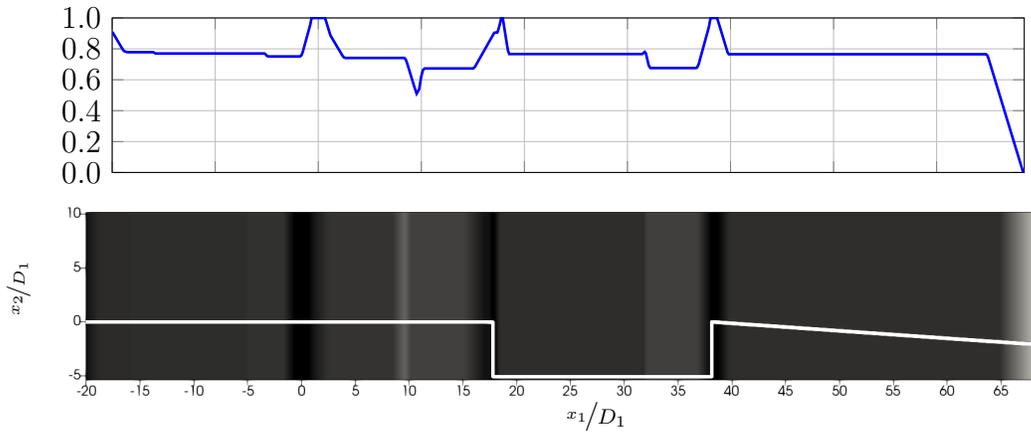
189 The corresponding computational grid features approximately 42,000,000 points and it
 190 is refined at some locations including the vicinity of walls, the hydrogen jet exit, and the
 191 shear layer that develops above the cavity. The characteristic dimensions of the resulting
 192 computational grid elements remain bounded between 15 μm and 275 μm , see Table 1.

	Δx_1 (m)	Δx_2 (m)	Δx_3 (m)
Min value	$5.0 \cdot 10^{-5}$	$1.5 \cdot 10^{-5}$	$5.0 \cdot 10^{-5}$
Max value	$1.475 \cdot 10^{-3}$	$4.062 \cdot 10^{-4}$	$2.478 \cdot 10^{-4}$
Average value	$2.711 \cdot 10^{-4}$	$2.387 \cdot 10^{-4}$	$1.865 \cdot 10^{-4}$

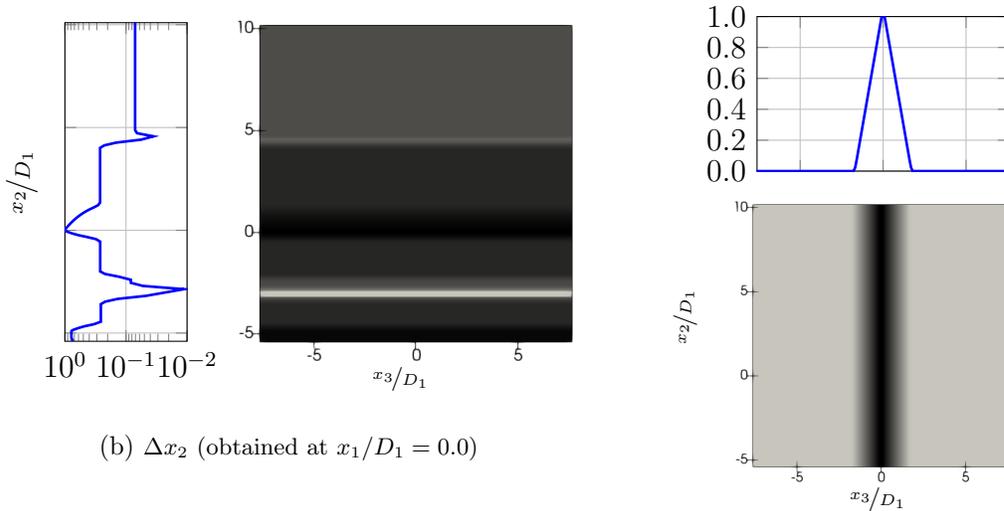
Table 1: Characteristic dimensions of the computational grid

193 A normalized mesh concentration parameter Δx_i^* is introduced to follow the spatial dis-
 194 cretization evolution with respect to its smallest and largest characteristic dimensions along
 195 each of the three directions. It is evaluated from $\Delta x_i^* = (\Delta x_{i,max} - \Delta x_i) / (\Delta x_{i,max} - \Delta x_{i,min})$,
 196 where Δx_i^* is the mesh concentration parameter, Δx_i the current (i.e., local) computational
 197 grid size, $\Delta x_{i,min}$ its smallest value, and $\Delta x_{i,max}$ its largest value. Thus, the value of Δx_i^*
 198 ranges between zero, for small concentration of computational nodes (i.e., large characteris-
 199 tic mesh dimension), and unity, for high concentration of computational nodes (i.e., small char-
 200 acteristic mesh dimension). Figure 2 reports the normalized mesh concentration Δx_1^* , Δx_2^* ,
 201 and Δx_3^* along the three spatial directions. It is noteworthy that the mesh origin has been set
 202 at the center of the fuel injection exit diameter. The bottom wall, including the wall-mounted
 203 cavity geometry, is modelled using the IBM. Except for the fuel inlet boundary condition (BC),

204 which is set as a supersonic inlet BC, the corresponding boundary condition is processed as a
 205 solid (i.e., impermeable) adiabatic wall with the energy and scalar zero-flux Neumann bound-
 206 ary conditions imposed using the GPF framework, and the zero-velocity Dirichlet boundary
 207 condition (i.e., no-slip wall) imposed through the combined GPF-DF framework, see Boukhar-
 208 fane et al. (2018) for further details. On the left side of the computational domain, the vitiated
 209 air inlet boundary condition is set as a supersonic inlet BC. The lateral and top boundaries
 210 are processed as slip walls. Finally, on the right side of the computational domain, the su-
 211 personic outlet is processed using extrapolation together with an additional sponge region
 212 combining both grid coarsening and explicit filtering, thus following the strategy previously
 213 retained by Buttay et al. (2016, 2017). Further details about the fuel and vitiated air inlet
 214 conditions are provided below.



(a) Δx_1 (obtained at $x_3/D_1 = 0.0$)



(b) Δx_2 (obtained at $x_1/D_1 = 0.0$)

(c) Δx_3 (obtained at $x_1/D_1 = 0.0$)

Figure 2: Normalized mesh size distributions with the cavity geometry delineated with a white line

	case RFSC-LST		case RFSC-HST	
	fuel	vitiated air	fuel	vitiated air
p (kPa)	845.0	55.410	755.0	55.426
Y_{H_2}	1.0	0.0	1.0	0.0
Y_{O_2}	0.0	0.244	0.0	0.251
Y_{N_2}	0.0	0.671	0.0	0.607
$Y_{\text{H}_2\text{O}}$	0.0	0.085	0.0	0.142

Table 2: Hydrogen and vitiated air inlets characteristics

215 The initial air stagnation (i.e., total) pressure is $p_{t,0} = 590.0$ kPa and two distinct values
216 of the vitiated air total temperature are considered to study the combustion stabilization
217 process. It is 1100.0 K in the first case, hereafter referred to as case RFSC-LST, and 1400.0 K
218 in the second, hereafter referred to as case RFSC-HST. Fuel is injected sonically at room
219 temperature. Table 1 gathers the main parameters that characterize the fuel and vitiated
220 air inlet streams for both cases. Upstream of the left boundary of the present computational
221 domain, the air inlet flow has been accelerated by a Mach 2.2 nozzle and passed through the
222 isolator. With the objective of imposing vitiated air inlet temperature and velocity profiles as
223 realistic as possible, preliminary simulations of the airflow in the isolator have been conducted
224 for both conditions considering $M_0 = 2.2$ and $T_0 = 1100$ K for case RFSC-LST, and $M_0 = 2.2$
225 and $T_0 = 1400$ K for case RFSC-HST. The pressure at the inlet of the computational domain
226 is determined from an isentropic evolution, with the value of the heat capacity ratio γ being
227 set to 1.313 and 1.287 for cases RFSC-LST and RFSC-HST, respectively, thus resulting in
228 pressure values equal to 55.410 kPa and 55.426 kPa.

229 The unsteady viscous flows inside the isolator have been simulated with the same LES
230 solver (CREAMS). As emphasized above, the objective of these preliminary computations is only
231 to impose realistic mean profiles for both the temperature and velocity at the inlet of the main
232 simulations. Taking advantage of the results issued from these preliminary computations of
233 the isolator, the filtered temperature and velocity components are settled from the computed
234 profiles of the averaged temperature $\{\tilde{T}\}$ and velocity components $\{\tilde{u}_i\}$ obtained at the
235 outlet of the isolator. However, it should be acknowledged that, in comparison with some
236 previous studies, e.g., Kawai and Lele (2010), no special effort has been spent to represent
237 the unsteady (i.e., turbulent) features of the supersonic boundary layer at the inlet of the
238 main simulation. In Kawai and Lele (2010), a concurrent supersonic turbulent boundary
239 layer (STBL) simulation has been conducted by making use of rescaling and reintroduction
240 procedures. The inflow conditions for the main JISCF simulation were extracted from a
241 plane of the concurrent STBL simulation. Other strategies based on the use of synthetic inlet
242 turbulence generators could have been also retained to model the present fluctuating inflow
243 conditions but, previous analyses, see for instance Vedovoto et al. (2015), showed that, even
244 with properly set mean velocity and turbulence kinetic energy, the resulting flowfields still
245 remain very sensitive to the arbitrary choice of the synthetic turbulence model. Therefore, for
246 the purpose of the present study, which is focused on other specific issues, a simpler solution

247 has been chosen with no fluctuations imposed at the inlet boundary.

248 The fuel injection boundary layer is taken into account by setting the following velocity
249 profile $u(r, t) = f(t) \cdot [u_w - (U_1 - u_w) \operatorname{erf}((r - r_1)/(2.0 \alpha r_1))]$ with $\alpha = 0.05$, where U_1 denotes
250 the hydrogen inlet bulk flow velocity, u_w is the flow velocity in the direct vicinity of the wall,
251 r is the distance to the center of the fuel injection, and $r_1 = D_1/2.0 = 1.25$ mm is the
252 radius of the fuel injection port. The function $f(t) = 1.0 - \exp(-5.0 t/t_1)$ has been used to
253 avoid numerical instabilities that may arise when the mass flow rate is applied directly. In
254 this expression, $t_1 = 0.2 \mu\text{s}$ is the characteristic time required for the injection to be fully
255 established.

256 Time is made non-dimensional by considering its product with the ratio of the fuel injection
257 port diameter D_1 to the fuel inlet bulk flow velocity U_1 . The simulations are started at
258 $t^* = U_1 t/D_1 = 0.0$ without any fuel injection and are run without any chemical reaction
259 until the fuel injection is developed in the whole computational domain. A typical snapshot
260 depicting an iso-surface ($\tilde{\xi} = 0.5$) of the fuel inlet tracer¹ is presented in Fig. 3. Chemical
261 reactions are then activated at $t^* = 300.0$, i.e., after a fuel particle got enough time to cross
262 the entire computational domain, and the simulation is run up to $t^* = 1200.0$. Datafiles are
263 stored at a frequency 1.0 MHz. During the numerical simulations, the CFL number value
264 has been varied between 0.3 and 0.7, while the Fourier number Fo has been set constant and
265 equal to 0.9.

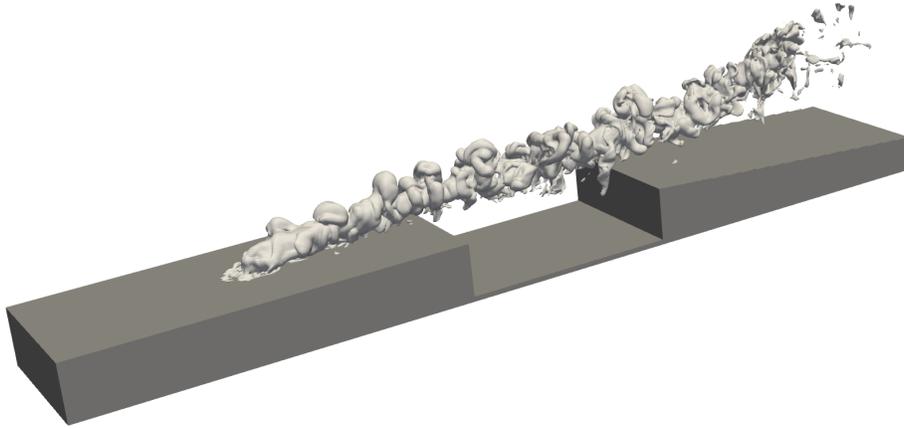


Figure 3: Iso-surface ($\tilde{\xi} = 0.5$) of the fuel inlet tracer at time $t^* = 350.0$ (case RFSC-LST)

266 4. Mesh reliability analysis

267 The retained numerical schemes together with the choice of SGS modelling closures, see
268 section 2, are well-known to be essential ingredients of any LES computations (Garnier et al.,
269 2009). They do not, however, constitute the sole issues that must be properly addressed: it
270 is indeed also worth recalling that the computational resolution is itself of the utmost im-
271 portance. For instance, in wall-bounded flows such as those considered herein, the integral

¹This quantity will be further discussed in the next section.

272 scale, away from the walls, is proportional to the turbulent boundary-layer thickness and
 273 the resolution requirement is determined by the range of scales contributing to the desired
 274 statistics. Mostly, the turbulent kinetic energy production results from high-speed streaks,
 275 which remain confined within a very small region in the direct vicinity of the wall (Kline
 276 et al., 1967). The corresponding flow structures are extremely small when compared to the
 277 overall flow dimensions. These small structures, however, play an essential role in the tur-
 278 bulent boundary layer dynamics and therefore need to be well resolved. The design of the
 279 computational mesh and associated levels of resolution thus result from a compromise be-
 280 tween turbulent dynamics reproduction and CPU costs. Based on the non-reactive computed
 281 flowfields, the present section will provide a detailed mesh reliability analysis. In this respect,
 282 it must be acknowledged that obtaining a strict proof of computational resolution adequacy
 283 remains quite challenging and instead, as documented in the present section, one can gather
 284 various clues that all bring support to the mesh quality assessment analysis. The conclusion
 285 drawn from this mesh reliability analysis will be confirmed by the subsequent inspection of
 286 the computed reactive flows.

	DNS	wall-resolved LES
Δx^+	10 – 15	50 – 150
Δy^+	1	< 2
Δz^+	5	10 – 40

Table 3: Recommended computational mesh size in wall units (Piomelli and Chasnov, 1996; Pope, 2000; Piomelli and Balaras, 2002)

287 There exist many criteria to asses the mesh resolution quality. Some of them are based
 288 on mathematical estimates, while others rely on rather heuristic arguments. For instance,
 289 Table 3 presents recommended orders of magnitude of computational mesh cell sizes for both
 290 DNS and wall-resolved LES computations. In this table, the values of Δx^+ , Δy^+ , and Δz^+
 291 denote the dimensions of the computational cells present at the wall location expressed in wall
 292 units, i.e., $\Delta x^+ = \Delta x_1/l_w$, $\Delta y^+ = \Delta x_2/l_w$, and $\Delta z^+ = \Delta x_3/l_w$. We recall that the wall char-
 293 acteristic length scale l_w is given by $l_w = \mu_w/\sqrt{\rho_w\tau_w}$, where $\tau_w = \mu_w (\partial \langle u_1 \rangle / \partial x_2)_w$ denotes
 294 the stress at the wall with $\langle u_1 \rangle$ the statistically-averaged value of the longitudinal velocity
 295 component (Lesieur et al., 2005). It is noteworthy that this value is presently estimated from
 296 the average of the filtered velocity component.

297 Figure 4 reports the distributions of the dimensions of the computational cells present at
 298 the wall location, expressed in wall units. The top subfigure, i.e., Fig. 4a, corresponds to dis-
 299 tributions obtained for case RFSC-LST, while the distributions obtained for case RFSC-HST
 300 have been gathered in the bottom subfigure, i.e., Fig. 4b. Since the focus of the present study
 301 is placed on the reactive flow development, these distributions correspond to values obtained
 302 in cells where the filtered mixture fraction $\tilde{\xi}$ is such that $0.001 \leq \tilde{\xi} \leq 0.999$, thus exclud-
 303 ing non-reactive mixtures associated to pure fuel or pure oxidizer. The inspection of these
 304 distributions confirms that the wall-resolved LES criteria of Table 3 are quite satisfactorily
 305 fulfilled.

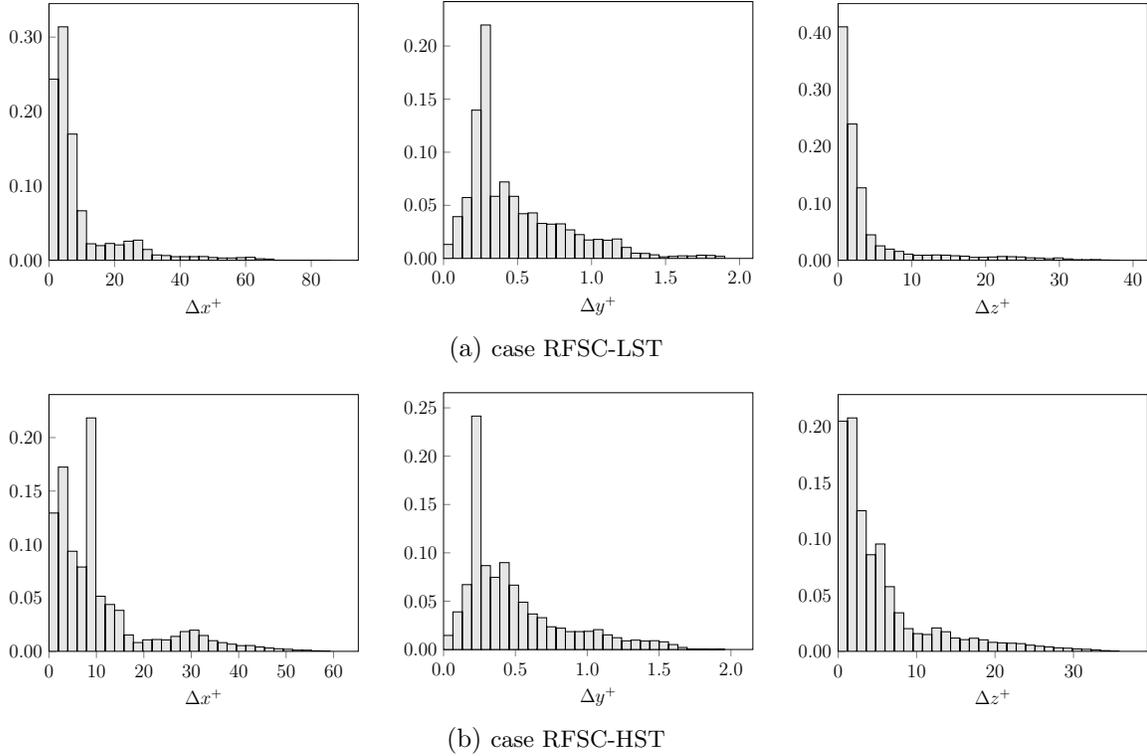


Figure 4: Normalized computational mesh size histograms

306 The mesh resolution quality in the vicinity of the walls is then assessed through a more
 307 detailed analysis of the averaged boundary layer flow. To this purpose, we consider again
 308 normalized quantities. In this respect, the longitudinal component of the non-dimensional
 309 mean velocity is defined by $\langle u_1 \rangle / u_{\tau_w}$ with $u_{\tau_w} = \sqrt{\tau_w / \rho_w}$ the wall friction velocity. Figure 5
 310 displays the profiles, in wall units, of the normalized mean velocity u^+ together with the
 311 logarithm of the viscosity ratio, i.e., $\log(\mu_{\text{SGS}} / \langle \tilde{\mu} \rangle)$, plotted versus the distance to the wall
 312 at several locations x_1 / D_1 . Here, the mean values have been obtained from an average
 313 performed over instantaneous snapshots of the median plane (i.e., $x_3 / D_1 = 0.0$). Despite the
 314 visible shift of the velocity in the logarithmic zone, these profiles confirm that the WALE
 315 model satisfactorily changes its behavior in the buffer layer that separates the logarithmic
 316 zone ($y^+ > 30.0$) from the viscous sublayer ($y^+ < 5.0$). Moreover, once plotted in logarithmic
 317 coordinates, the viscosity ratio increases almost linearly, which is consistent with its expected
 318 behavior (Nicoud and Ducros, 1999; Techer et al., 2018).

319 The assessment of the computational resolution is completed through a detailed mesh
 320 quality analysis. In this purpose, two quality indexes are considered. The corresponding
 321 quantities vary from zero (i.e., poor mesh resolution) to unity (i.e., good mesh resolution):
 322 the higher the value of the index, the better the resolution. First, we consider the modified
 323 quality index of Pope (2004), which is defined as follows: $\text{IQ}_k = k / (k + k_{\text{SGS}})$, where k denotes
 324 the resolved turbulent kinetic energy and k_{SGS} is its subgrid-scale unresolved counterpart,
 325 which is presently evaluated from the Yoshizawa closure $k_{\text{SGS}} = \nu_{\text{SGS}} / (C_M \Delta)^2$ with $C_M =$

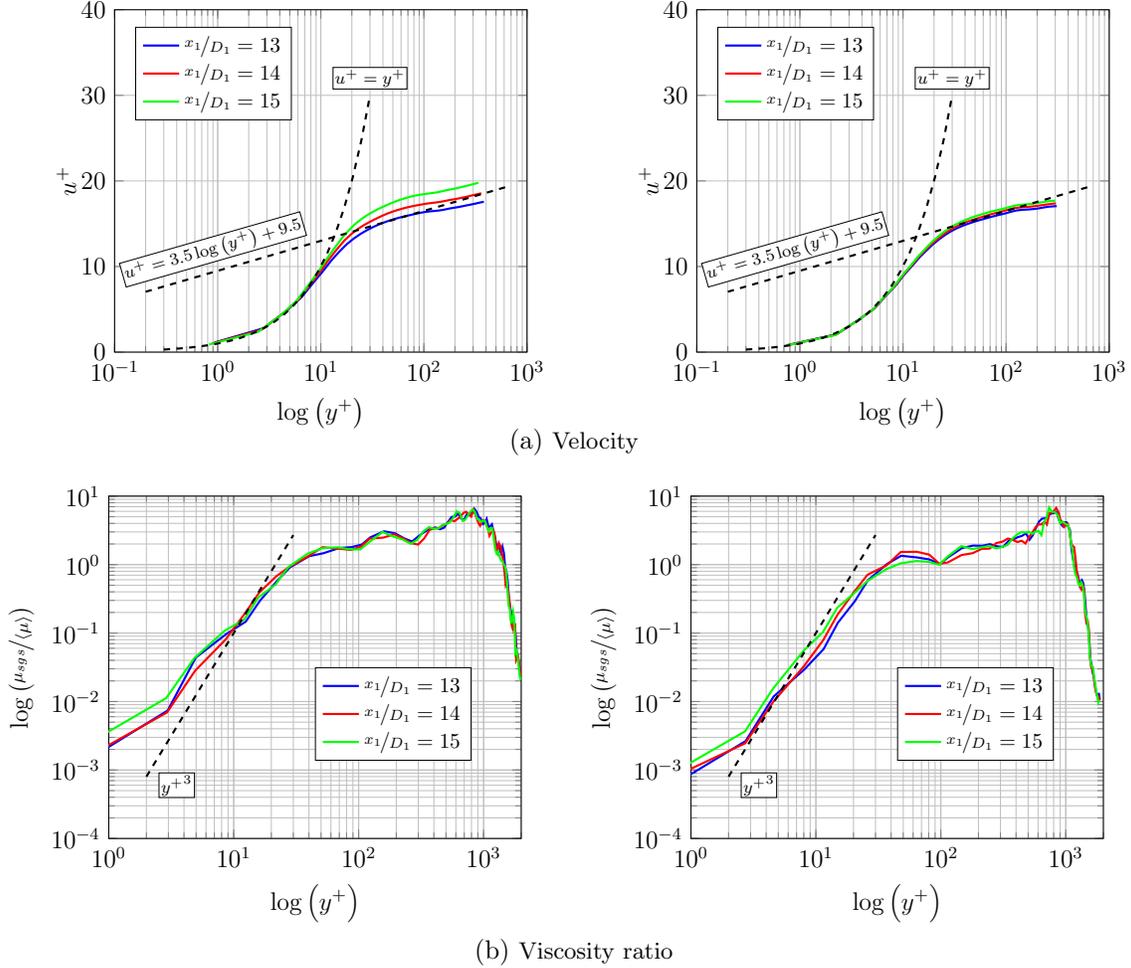


Figure 5: Non dimensional velocity profile in wall units and viscosity ratio profile at several locations x_1/D_1 for cases RFSC-LST (left) and RFSC-HST (right)

0.069 (Yoshizawa, 1986). According to Pope (2004), the mesh resolution could be considered as sufficient, provided that the value IQ_k exceeds 0.80, which means that at least eighty percent of the turbulent kinetic energy is captured at the resolved scale. However, this quality index may display some sensitivity to the SGS modelling and, therefore, it seems worthwhile to complete the analysis with other estimates. To this purpose, the quality index of Celik et al. (2005) is also considered. It is based on a comparison between the computational grid characteristic size and the Kolmogorov length scale, as given by $IQ_\eta = (1 + \alpha_\eta(\Delta/\ell_\eta)^m)^{-1}$, with $(\alpha_\eta, m) = (0.05, 0.5)$ and ℓ_η evaluated from the following scaling rule $\ell_\eta = (\nu^3/\varepsilon)^{1/4}$ with ε being the turbulent kinetic energy dissipation rate. In this respect, it seems worth recalling that a standard criterion for DNS computation is $k_{max} \cdot \ell_\eta = 3/2$ in such a manner that, approximating k_{max} from π/Δ (Pope, 2000), it leads to a value of Δ/ℓ_η approximately equal to 2.0. Once introduced in the expression of the quality index IQ_η , this gives $IQ_\eta = 0.93$. This means that, in regions characterized by $IQ_\eta \geq 0.93$, the computational resolution can be considered as equivalent to the fulfillment of a standard DNS resolution criterion.

Figure 6 displays the probability density function (PDF) of the two quality indexes ob-

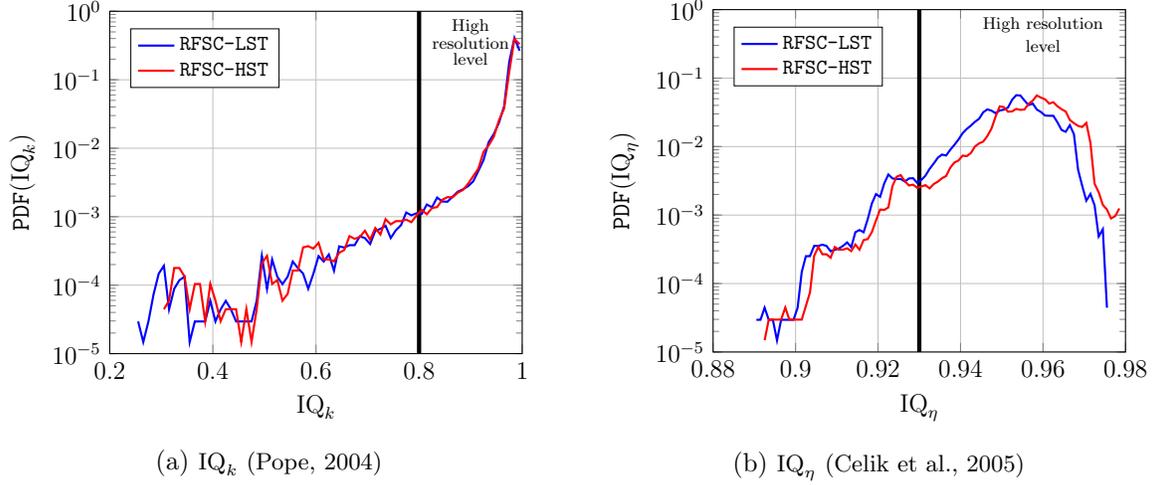


Figure 6: PDF of the quality index obtained in the median plane along the spanwise direction (i.e., $x_3/D_1 = 0.0$)

341 tained in the medium plane ($x_3/D_1 = 0.0$) of the computational mesh. The corresponding
 342 statistics show that most of the obtained values of the quality index IQ_k (resp. IQ_η) are larger
 343 than 0.80 (resp. 0.93). This conclusion can be more firmly and quantitatively assessed from
 344 a direct inspection of the cumulative distribution function (CDF), the expression of which is
 345 given by

$$\mathbb{F}(x) = \int_0^x \text{PDF}(IQ) \, dIQ \quad (11)$$

346 and its complement to unity

$$1 - \mathbb{F}(x) = 1 - \int_0^x \text{PDF}(IQ) \, dIQ = \int_x^1 \text{PDF}(IQ) \, dIQ \quad (12)$$

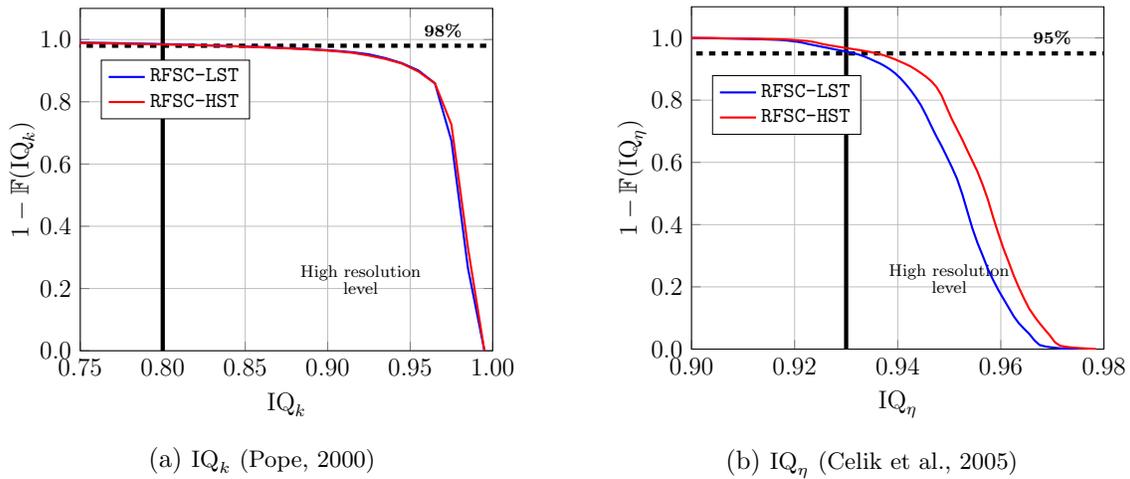


Figure 7: Value of $1 - \mathbb{F}(IQ)$, i.e., value of the probability to have a quality index larger than IQ . The probability to reach a level of the quality index larger than 0.80 for IQ_k and larger than 0.93 for IQ_η are also delineated.

347 The second expression, i.e., the one provided by Eq. (12), measures the probability of

348 having a value of the quality index IQ larger than x . Figure 7 thus shows that almost 98% of
 349 the values of the Pope quality index IQ_k are larger than 0.80. It also reveals that 95% of the
 350 values of the quality index IQ_η are larger than 0.93, a value that corresponds to the standard
 351 DNS resolution requirement discussed above.

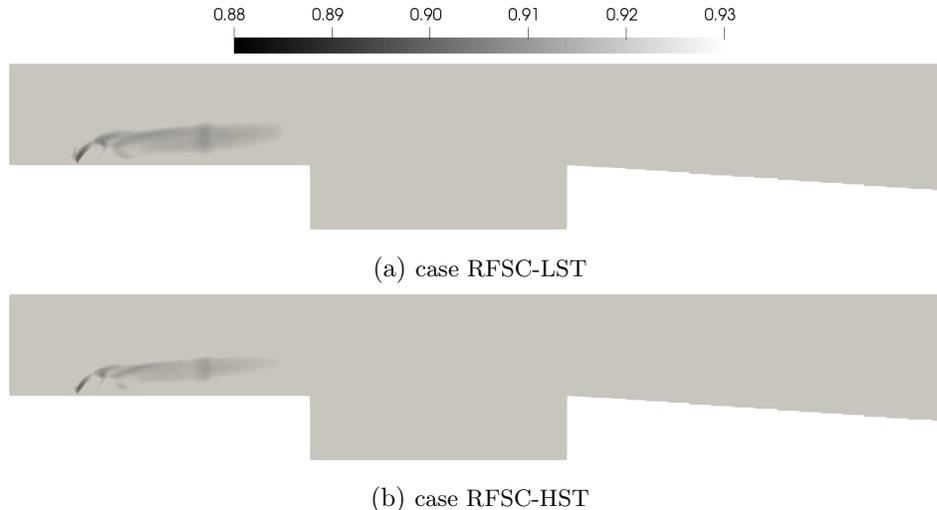


Figure 8: Mean fields of the index IQ_η obtained in the median plane along the spanwise direction ($x_3/D_1 = 0.0$)

352 Finally, Fig. 8 reports the mean field of IQ_η obtained in the median plane along the
 353 spanwise direction ($x_3/D_1 = 0.0$). This figure confirms that the vicinity of the fuel injection
 354 and the shear layer that develops above the wall-mounted cavity display quite satisfactory
 355 levels of resolution. The resolution level is also excellent upstream of the fuel inlet port and
 356 only slightly decreases downstream of the hydrogen injection; even in this region, the values
 357 of IQ_η indeed remain such that $IQ_\eta \geq 0.90$. The inference from all the quantities discussed
 358 above is that the present set of computations indeed displays a high level of resolution. As
 359 summarized in section 2, this high level of resolution is combined with the use of high-precision
 360 numerical schemes and subgrid-scale models that satisfactorily recover the DNS limit, thus
 361 resulting in solid bases to perform high-fidelity numerical simulations.

operator	definition
$\bar{\Phi}$	(spatially-) filtered value
$\tilde{\Phi} = \overline{\rho\Phi}/\bar{\rho}$	(spatially-) Favre-filtered value
$\langle \Phi \rangle$	(temporal-) averaged value
$\{\Phi\} = \langle \rho\Phi \rangle / \langle \rho \rangle$	(temporal-) Favre-averaged value

Table 4: Expressions of spatial filtering and temporal averaging operators

362 Finally, it must be underlined that the targeted objective is the simulation of the reactive
 363 flow stabilization and we are not really interested by the description of the flow inside the
 364 exit nozzle. Therefore, the mesh has been considerably coarsened in this region of the com-
 365 putational domain and no special effort has been spent to describe the flow in this part of the

366 combustor. As a consequence, there are some pressure disturbances that appear at the nozzle
 367 wall at the level of each cell transition. The birth of such perturbations in the exit nozzle is
 368 visible on numerical schlieren images and has been already reported in the literature when
 369 coarse meshes are considered.

370 5. Analysis of computational results

371 5.1. Statistical convergence of the computational datasets

372 Before proceeding with a detailed inspection of the computational results, we proceed
 373 with a statistical convergence analysis. Therefore, in an attempt to verify the convergence of
 374 the second-order moments of the velocity field, eight probes are placed in the median plane
 375 of the computational domain (i.e., $x_3/D_1 = 0.0$), as depicted in Fig. 9. Table 4 summarizes
 376 the various spatial filtering and temporal averaging operators. At this level, it should be
 377 emphasized that, for the present application to LES data, the temporal operator is applied
 378 to filtered quantities. For instance, the temporal average of the density is evaluated from the
 379 resolved density field using $\langle \bar{\rho} \rangle$.

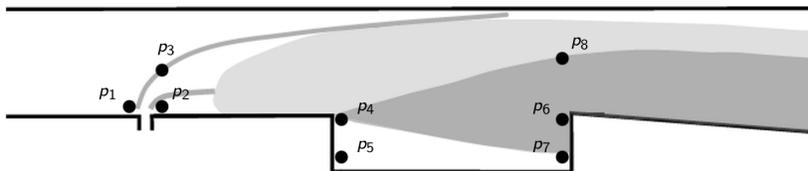


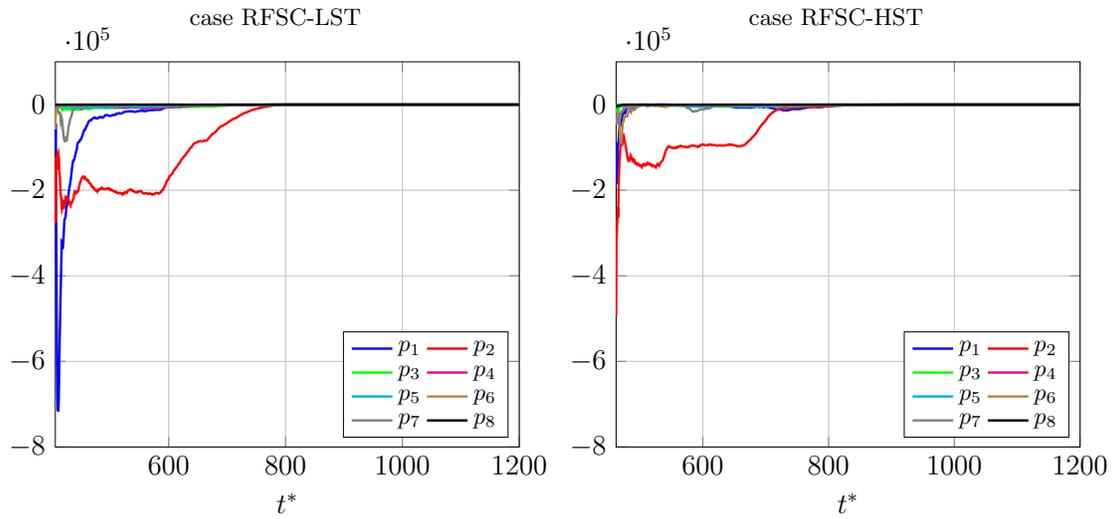
Figure 9: Probes location for the second-order moments convergence verification

380 Recalling that the second-order centered moment of any quantity Φ is the expected value
 381 of the squared deviation from its mean, i.e., $\sigma_{\Phi}^2 = \langle (\Phi - \langle \Phi \rangle)^2 \rangle = \langle \Phi^2 \rangle - \langle \Phi \rangle^2$, the tem-
 382 poral convergence of the second-order moments of the filtered velocity field \tilde{u}_i is checked by
 383 evaluating the following expression:

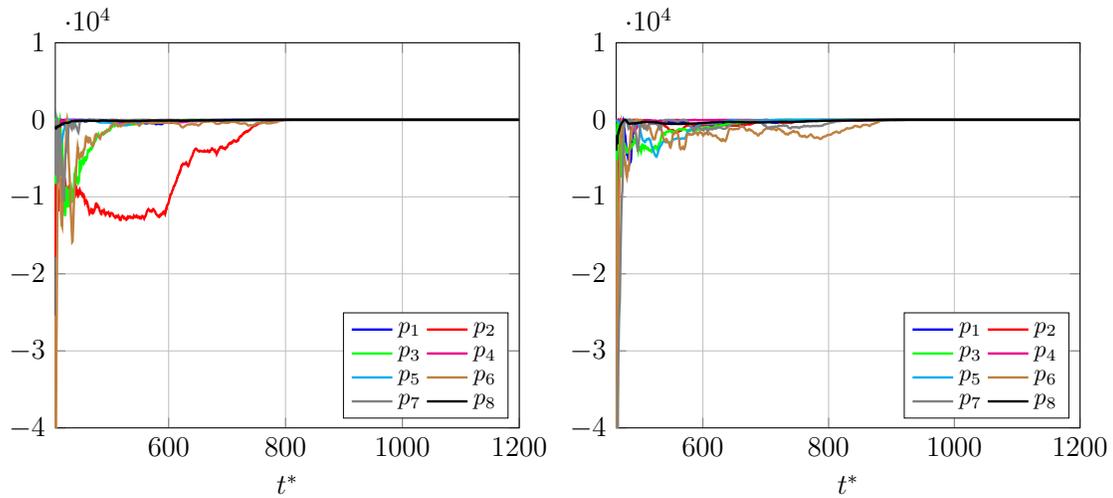
$$R_{\tilde{u}_i} = \langle \tilde{u}_i \tilde{u}_i \rangle - \langle \tilde{u}_i \rangle \langle \tilde{u}_i \rangle - \langle (\tilde{u}_i - \langle \tilde{u}_i \rangle)^2 \rangle \quad (13)$$

384 The above quantity, i.e., the residual $R_{\tilde{u}_i}$, should be zero provided that $\langle \langle \tilde{u}_i \rangle \langle \tilde{u}_i \rangle \rangle = \langle \tilde{u}_i \rangle \langle \tilde{u}_i \rangle$
 385 and $\langle \langle \tilde{u}_i \rangle \tilde{u}_i \rangle = \langle \tilde{u}_i \rangle \langle \tilde{u}_i \rangle$, which provides an excellent verification of the convergence of the
 386 temporal averaging operator.

387 Figure 10 displays the statistical convergence of the longitudinal and transverse compo-
 388 nents of the velocity field for cases RFSC-LST and RFSC-HST as obtained on the various
 389 probes defined in Fig. 9. From these results, one can notice that the solution convergence is
 390 obtained for $t^* \geq 800.0$ and $t^* \geq 900.0$ for cases RFSC-LST and RFSC-HST, respectively.
 391 Therefore, the statistical post-processing of the computational results will be performed over
 392 snapshots obtained from these values up to the end of the simulation.



(a) Second-order residual of the longitudinal filtered velocity component $R_{\tilde{u}_1}$

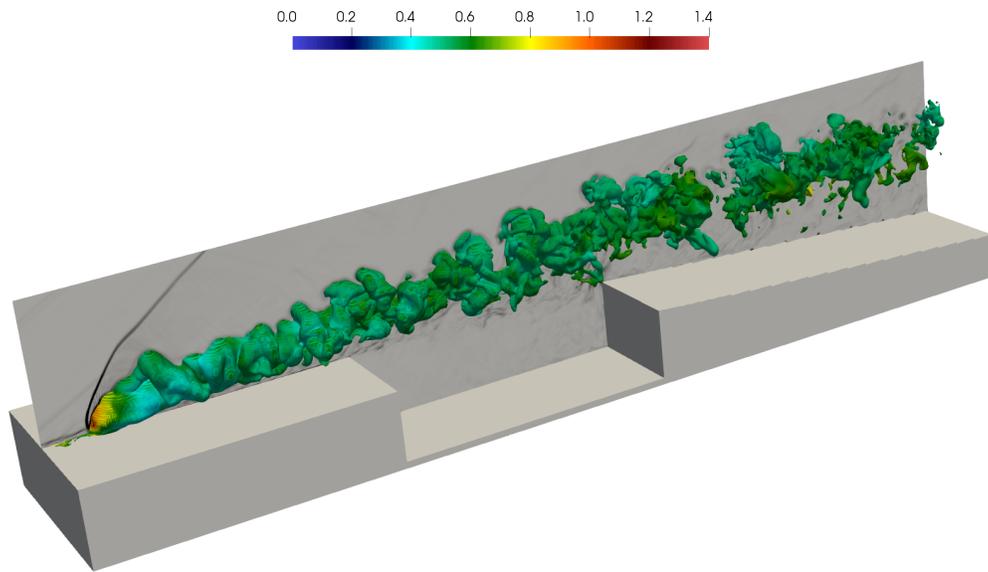


(b) Second-order residual of the transverse filtered velocity component $R_{\tilde{u}_2}$

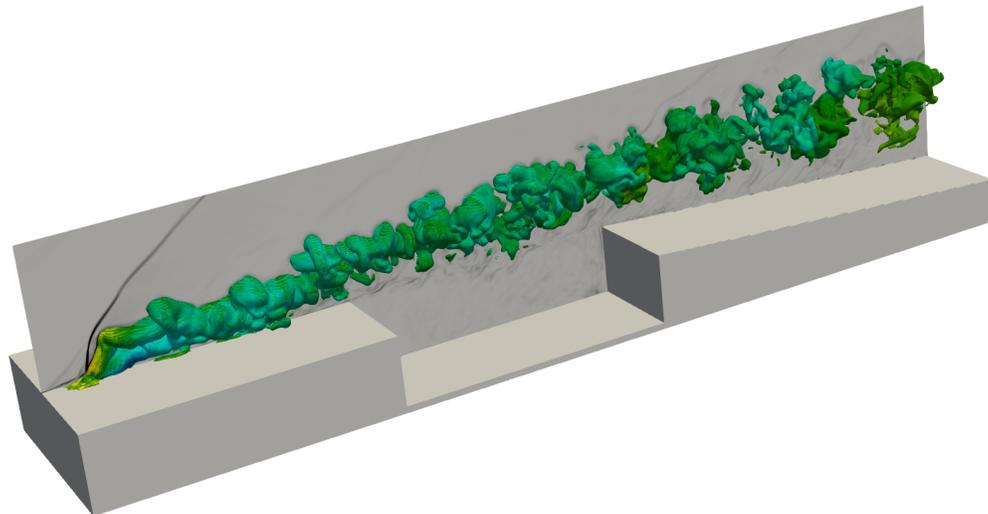
Figure 10: Convergence of the second-order moments of filtered velocity at the probe locations defined in Fig. 9

393 *5.2. Non-reactive flow analysis*

394 Figure 11 displays an instantaneous numerical Schlieren image in the median plane to-
 395 gether with an iso-surface of the fuel mass fraction ($\tilde{Y}_{\text{H}_2} = 0.5$) colored by the normalized
 396 filtered temperature field \tilde{T}/T_0 for cases RFSC-LST and RFSC-HST. The topology of JISCF
 397 compressible flowfield has been largely discussed in the literature for both non-reactive (Kawai
 398 and Lele, 2010) and reactive conditions (Ben Yakar and Hanson, 1998). The hydrogen un-
 399 derexpanded jet quickly expands through a Prandtl-Meyer fan at the boundary of the jet
 400 orifice prior to being compressed through a barrel shock and a Mach disk. The jet forms two
 401 series of counter-rotating vortices the rotation axis of which are aligned with the downstream
 402 direction. At the fuel injection location, the supersonic vitiated airstream is blocked by the



(a) case RFSC-LST

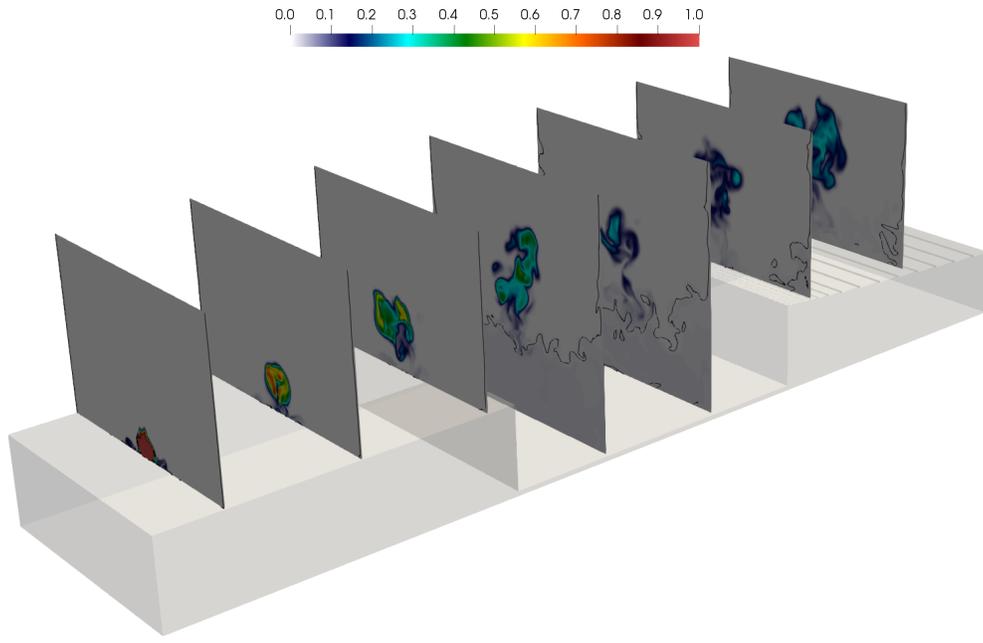


(b) case RFSC-HST

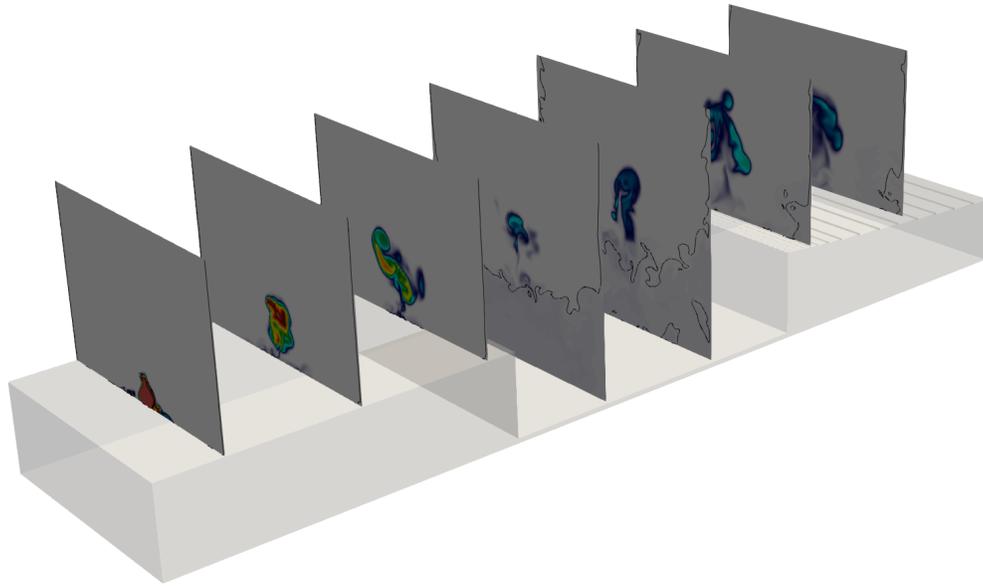
Figure 11: Instantaneous numerical Schlieren in the median plane together with an iso-surface of the fuel mass fraction colored by the normalized temperature field

403 highly underexpanded² transverse jet of hydrogen, with compression waves leading to the
 404 birth of a three-dimensional bow shock created ahead of the jet. It causes boundary layer
 405 separation and leads to the formation of a horseshoe vortex region downstream of the jet.
 406 The mixing process mainly takes place downstream of the barrel shock because there is a very
 407 high velocity gradient between the hydrogen jet and the crossflow. This triggers the birth of
 408 large-scale coherent structures induced by the Kelvin-Helmholtz (K-H) instabilities. Further
 409 downstream, the scale reduction processes come into play, thus leading to the breakup of these

²The nozzle pressure ratio (NPR) is larger than ten.



(a) case RFSC-LST



(b) case RFSC-HST

Figure 12: Instantaneous contours of fuel mass fraction together with the sonic iso-line (in black) in several spanwise planes

410 large-scale vortices.

411 Figure 12 reports instantaneous contours of fuel jet mass fractions together with the sonic
 412 iso-line in several spanwise planes. The mixing between fuel and oxidizer starts at the fuel
 413 jet injection with most of the fuel spread into the supersonic flow. The fuel jet is however
 414 slightly torn up by the cavity low-speed flow, with a small part of the hydrogen flowing into
 415 the wall-mounted cavity, which should result in some mixing enhancement due to recirculation
 416 zones present in the cavity. This may be checked through a mixing efficiency analysis.

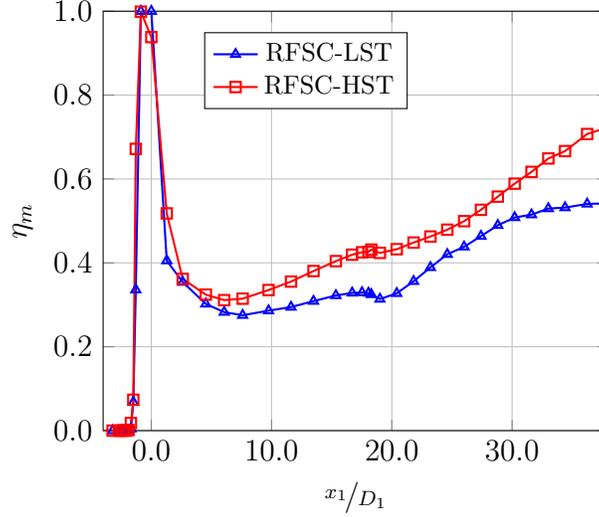


Figure 13: Mixing efficiency profile along the streamwise direction. The wall-mounted cavity extends from $x_1/D_1 = 17.8$ to $x_1/D_1 = 38.1$.

417 The corresponding fuel mixing degree is indeed a critical parameter to evaluate the super-
 418 sonic combustor performance as a whole. In this respect, there exist many possible definitions
 419 of the mixing efficiency in the literature, see for instance Moule et al. (2014b) and Liu et al.
 420 (2017). This quantity, i.e., the fuel mixing degree, can be defined as the mass flow rate ratio
 421 of reactants that would react to the total mass flow rate of reactants (Liu et al., 2017):

$$\eta_m(x_1) = \int_{\mathcal{A}(x_1)} \bar{\rho} \tilde{u}_1 Y_{\text{H}_2,r} dA / \int_{\mathcal{A}(x_1)} \bar{\rho} \tilde{u}_1 \tilde{Y}_{\text{H}_2} dA \quad (14)$$

422 where, following Liu et al. (2017), the mass fraction of reactants that would be involved in
 423 the reaction $Y_{\text{H}_2,r}$ is evaluated by assuming a complete oxidation of the available amount of
 424 hydrogen:

$$Y_{\text{H}_2,r} = \begin{cases} \tilde{Y}_{\text{H}_2} & \tilde{Y}_{\text{H}_2} \leq Y_{\text{H}_2,st} \\ Y_{\text{H}_2,st}(1 - \tilde{Y}_{\text{H}_2}) / (1 - Y_{\text{H}_2,st}) & \tilde{Y}_{\text{H}_2} \geq Y_{\text{H}_2,st} \end{cases} \quad (15)$$

425 with $Y_{\text{H}_2,st}$ the fuel mass fraction at stoichiometry. In Eq. (14), the elementary transverse
 426 surface element dA is evaluated from the product $\Delta x_2 \cdot \Delta x_3$ and, at each location x_1 , the
 427 integral is performed over the whole transverse section $\mathcal{A}(x_1)$.

428 Figure 13 displays the mixing efficiency profile obtained along the streamwise direction,
 429 zooming at the fuel injection and wall-mounted cavity, i.e., in a region delineated by $-4.0 \leq$
 430 $x_1/D_1 \leq 38.0$. The obtained results display some similarities with those previously reported
 431 by Liu et al. (2017) who retained the same definition of the mixing efficiency. Thus, the mixing
 432 efficiency is found to be close to 100% in the direct vicinity of the fuel injection, where only
 433 a small amount of fuel diffused along the turbulent boundary layer. A minimum is reached
 434 ahead of the fuel jet injection because the mixing is dominated by the large scale vortices in
 435 the jet shear layer. Then, the mixing efficiency increases faster along the cavity, which means
 436 that mixing processes are enhanced, reaching finally almost 100% at the end of the cavity.

437 The present set of non-reactive results is now used to perform an analysis of ignition
 438 probabilities. Mixtures of fuel and oxidizer are indeed considered to be flammable only if a
 439 premixed flame is able to propagate into the corresponding fresh reactants, which happens
 440 only within given composition limits. The flammability limits of a reactive mixture determine
 441 the lower and upper fuel concentration so that combustion can proceed. These values are
 442 obtained from well-defined experimental procedures by varying the mixture composition and
 443 they may be altered not only by temperature and pressure but also by flame propagation
 444 direction under a gravitational field (Zabetakis, 1965). The lowest fuel concentration that
 445 may lead to flame propagation is hereafter denoted as the lower flammability limit (LFL),
 446 while the largest fuel concentration is called the upper flammability limit (UFL). Both LFL
 447 and UFL are expressed in terms of volume percentages in normal conditions, i.e., at 298 K
 448 and 1.0 atm. For instance, the LFL and UFL values for mixtures of hydrogen with air
 449 are 4% and 75% (Zabetakis, 1965), which correspond to mixture fraction values equal to
 450 0.003 and 0.167, respectively. At this level, it should be emphasized that there exist several
 451 possible ways to evaluate the mixture fraction. Discarding Lewis number effects, i.e., assuming
 452 the mixture fraction molecular diffusion coefficient equal to thermal diffusivity, this quantity
 453 may be thought as a fuel inlet tracer (Gomet et al., 2015), the value $\tilde{\xi}_f$ of which can be
 454 evaluated from a filtered passive scalar transport equation with boundary conditions set to
 455 zero ($\tilde{\xi}_f = 0.0$) at the oxidizer inlet and unity ($\tilde{\xi}_f = 1.0$) at the fuel inlet. The mixture fraction
 456 can also be deduced from atoms conservation. For instance, the nitrogen mass fraction \tilde{Y}_{N_2} ,
 457 which has been considered as a non-reactive scalar in the present set of computations³, can
 458 be used to this purpose: $\tilde{\xi}_{N_2} = 1.0 - (\tilde{Y}_{N_2}/Y_{N_2}^{\max})$ with $Y_{N_2}^{\max}$ the nitrogen concentration in
 459 the vitiated airstream inlet. Finally, it is also possible to evaluate the mixture fraction on the
 460 basis of the chemical reaction stoichiometry (Peters, 2000):

$$\tilde{\xi} = \frac{\phi \left(\tilde{Y}_{H_2}/Y_{H_2}^\infty \right) - \left(\tilde{Y}_{O_2}/Y_{O_2}^\infty \right) + 1}{1 + \phi} \quad (16)$$

461 where $Y_{H_2}^\infty$ is the hydrogen mass fraction issued from the fuel inlet (unity in the present
 462 case of pure fuel injection), $Y_{O_2}^\infty$ is the oxygen mass fraction in the vitiated airstream, and
 463 $\phi = r_{st} \left(Y_{H_2}^\infty/Y_{O_2}^\infty \right)$ denotes the equivalence ratio with r_{st} the stoichiometric mass ratio. These
 464 various definitions are compared in Fig. 14, which reports the averaged profiles based on the
 465 use of each definition. For the present conditions, the obtained differences appear to be so
 466 slight that they can be neglected.

467 From the resolved mixture fraction PDF, the ignition probability P_{ign} may be evaluated
 468 as follows:

$$P_{ign} = \int_{0.003}^{0.167} \left\langle P \left(\tilde{\xi} \right) \right\rangle d\tilde{\xi} \quad (17)$$

469 The field of the corresponding ignition probability P_{ign} , obtained from the averaging of data
 470 obtained in the median plane ($x_3/D_1 = 0.0$), is reported in Fig. 15 for cases RFSC-LST

³It is indeed worth noting that nitrogen is not involved in the detailed chemistry description considered in the present study.

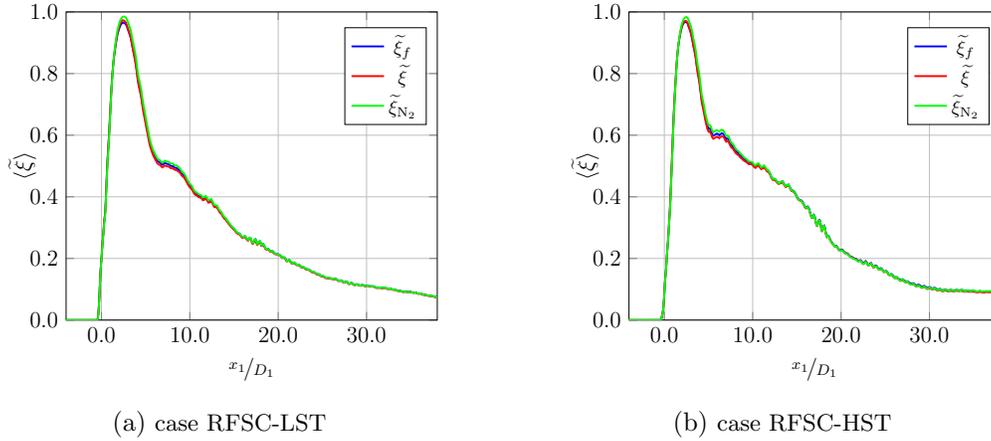


Figure 14: Averaged mixture fraction profiles obtained using three distinct definitions

471 and RFSC-HST. This view is restricted to a zoom for a close-up of the fuel injection and
 472 cavity regions. One can verify that, even with the present set of values of the flammability
 473 limits, which are associated to normal conditions (i.e., moderate temperature levels in the
 474 fresh reactants), the highest levels of the ignition probability P_{ign} follow quite closely the
 475 jet wake and the shear layer that develops above the cavity. It is interesting to notice that,
 476 in case RFSC-HST, there is a larger region featuring high values of P_{ign} in the vicinity of
 477 the wall downstream of the hydrogen injection. As it will be shown later on, these locations
 478 correspond to those where the jet-wake and cavity stabilization modes develop. However, it
 479 should be fairly acknowledged that the consideration of the operating temperature level of
 480 the vitiated airstream T_0 , instead of the temperature 298 K associated to normal conditions,
 481 may significantly alter the results and more insights should be gained from the reactive flow
 482 simulations presented in the next section.

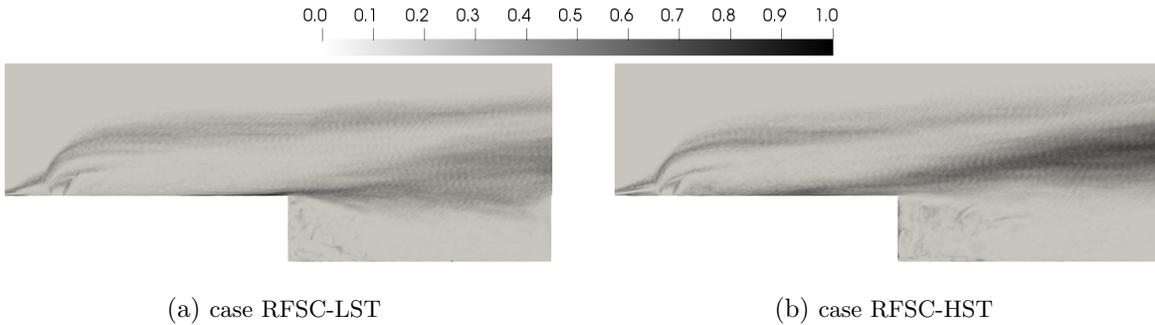


Figure 15: Ignition probability P_{ign} in the median plane $x_3/D_1 = 0.0$

483 5.3. Reactive flow analysis

484 According to the studies of Micka and Driscoll (2008), for the range of conditions reported
 485 in Micka's Thesis manuscript (Micka, 2010), the vitiated air-stream temperature T_0 plays an
 486 important role in determining the combustion stabilization mode. For inlet temperature such

487 that $T_0 > 1350$ K, combustion stabilization occurs through a jet-wake mode, whereas for
 488 $T_0 < 1150$ K, a cavity-stabilized regime is expected. In the intermediate range (1150 K <
 489 $T_0 < 1350$ K) combustion oscillates between the two stabilization regimes. Equation (18)
 490 may be used to approximate the fraction of time f the combustion takes place in jet-wake
 491 stabilized mode (Micka and Driscoll, 2008):

$$f = \frac{1}{2} + \frac{|T_0 - 1250.0|}{2} \operatorname{erf} \left(\frac{T_0 - 1250.0}{75.0} \right) \quad (18)$$

492 where the value of the vitiated airstream temperature T_0 must be provided in Kelvin S.I. unit.
 493 The corresponding function is displayed in Fig. 16 together with the two conditions studied
 494 in the present work.

495 From a practical viewpoint, the flame will remain in the cavity-stabilized mode for mod-
 496 erate values of the temperature T_0 except if a large enough fluctuation flashes it forward to
 497 a relatively stable location in the jet-wake stabilization region. If this occurs, the flame will
 498 then remain in the jet-wake stabilized mode until it becomes unstable due to another fluctua-
 499 tion, forcing it to flash back to a cavity-stabilized regime. The magnitude of the fluctuations
 500 required for the flame to flash back and forth becomes smaller as the temperature T_0 rises.
 501 Moreover, as T_0 is increased, the magnitude of the fluctuations that may cause the flame to
 502 flash back increases also. Thus, with the rise of the temperature T_0 , combustion spends more
 503 time in the jet-wake stabilized mode, until it reaches a sufficiently high level of temperature
 504 where it cannot be destabilized by any fluctuation.

505

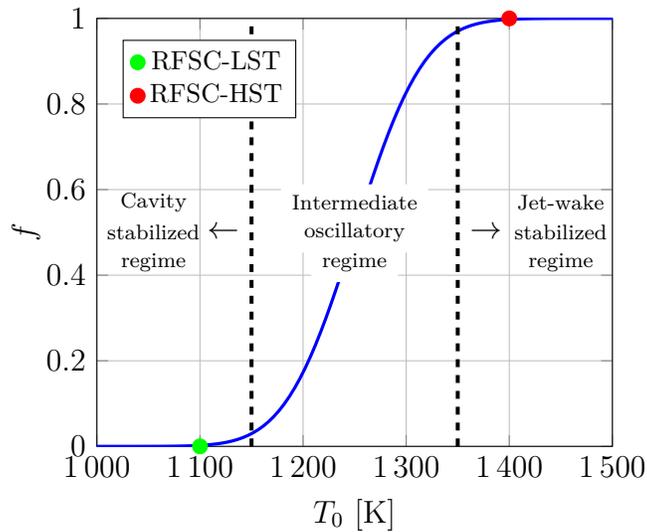


Figure 16: Combustion stabilization mode versus vitiated air-stream temperature

506 In the experiments, for obvious safety reasons, it is necessary to ensure that the ignition
 507 of the mixture will be successful and a spark plug located in the center of the cavity bottom
 508 wall is used. In the computations, ignition is simply obtained from the temperature increase
 509 on the rear wall of the cavity. As far as the use of adiabatic wall condition is concerned,

510 it seems worth to emphasize that, according to the information provided by Micka (2010),
 511 after the end of the main fuel injection (end of a given run), all flow streams except the main
 512 airstream were terminated and the electric heater was turned off. The main cold stream of
 513 air continued to flow through the combustor between two consecutive runs to provide cooling
 514 before the next test. According to Micka (2010), eight combustion tests can be performed
 515 in a day. In this manner, the possible influence of experimental condition variations between
 516 the runs remains limited. Finally, it is noteworthy that the same adiabatic condition has
 517 been retained in the other (seldom) computational studies of this experimental setup, see for
 518 instance Zettervall and Fureby (2018).

519 In a first step of the reactive flow analysis, a comparison is performed between computa-
 520 tional results obtained using either the PSR or the U-PaSR subgrid-scale combustion models.
 521 Such a comparison may be useful to further assess the level of computational resolution. The
 522 PSR model corresponds to the quasi-laminar approximation and consists in neglecting the
 523 possible influence of subgrid-scale fluctuations at the resolved level: the filtered reaction rates
 524 are evaluated directly from the detailed chemical scheme applied to the filtered composition.
 525 The PSR, i.e., well-stirred reactor (WSR), and PaSR representations are standardly retained
 526 as elementary building blocks of supersonic combustion modelling (Gomet et al., 2012; Pot-
 527 turi and Edwards, 2015; Fulton et al., 2016; Candler et al., 2017). In the present study,
 528 the U-PaSR modelling framework has been also considered (Moule et al., 2014a). Like the
 529 eddy-dissipation concept (EDC) model (Ertesvag and Magnussen, 2000), the U-PaSR is a
 530 multiscale-based model that takes into account the inhomogeneities of the composition vector
 531 $\psi = [T, Y_\beta]$ (i.e., temperature and species mass fractions) in the flame region, considering
 532 the effects of micro-mixing, finite-rate chemistry, and the interactions between them. Non-
 533 premixed combustion is assumed to take place in small dissipative structures (i.e., worms)
 534 where molecular mixing processes, which are a prerequisite before chemical reactions occur,
 535 are the most intense. It can be shown that the filtered chemical reaction rate can be ex-
 536 pressed as follows: $\bar{\Omega}_\alpha = \bar{\rho} \tilde{\omega}_\alpha = \gamma^* \bar{\Omega}_\alpha(\psi^*)$, where $\psi^* = [T^*, Y_\beta^*]$ denotes the composition of
 537 the highly dissipative fine-scale structures and γ^* measures their volume fraction. It can be
 538 shown that the U-PaSR closure recovers the DNS limit as the filter size Δ tends to zero (Moule
 539 et al., 2014a). Indeed, as $\Delta \rightarrow \epsilon$, with ϵ any arbitrary small number, we have $\gamma^* \rightarrow 1.0$ and
 540 $\psi^* \rightarrow \bar{\psi} = \psi$ and, as a result, $\bar{\Omega}_\alpha = \Omega_\alpha(T, Y_\beta)$. The SGS combustion model degenerates to
 541 its DNS counterpart, i.e., the instantaneous Arrhenius laws that are involved in the detailed
 542 chemical scheme.

543 Figures 17 and 18 report, respectively, the averaged cross stream profiles of OH and
 544 HO₂ mass fractions obtained at several locations x_1/D_1 , considering the PSR (blue line) and
 545 the U-PaSR (red line) SGS model, for cases RFSC-LST (continuous line) and RFSC-HST
 546 (dashed line). From this figure, it is clear that the PSR and U-PaSR models lead to quite
 547 similar results. This is an outcome of the well-resolved computational meshes, which lead the
 548 subgrid-scale U-PaSR model to behave like a perfectly-stirred reactor (PSR). In the regions
 549 where chemical reactions take place, the field of γ^* — not reported for the sake of conciseness
 550 — is indeed found to approach unity and it remains larger than 0.85 as a whole. The PSR or

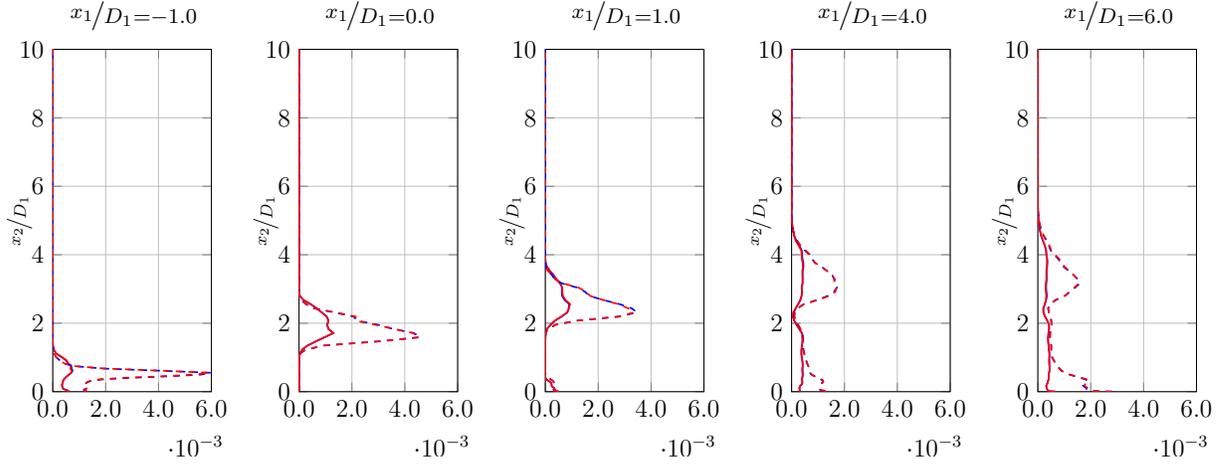


Figure 17: PSR (blue) and U-PaSR (red) OH averaged mass fraction profile comparison, for cases RFSC-LST (continuous line) and RFSC-HST (dashed line)

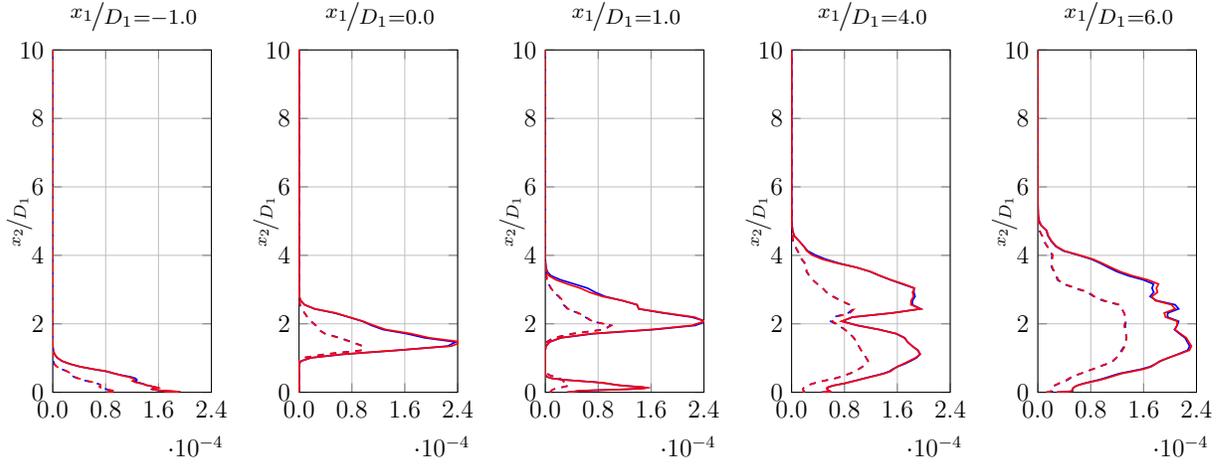


Figure 18: PSR (blue) and U-PaSR (red) HO₂ averaged mass fraction profile comparison, for cases RFSC-LST (continuous line) and RFSC-HST (dashed line)

551 quasi-laminar approximation thus appears as a relevant representation of chemical reactions
 552 in the present conditions, and the next steps of the discussion will therefore be restricted to
 553 computational results obtained with the PSR model.

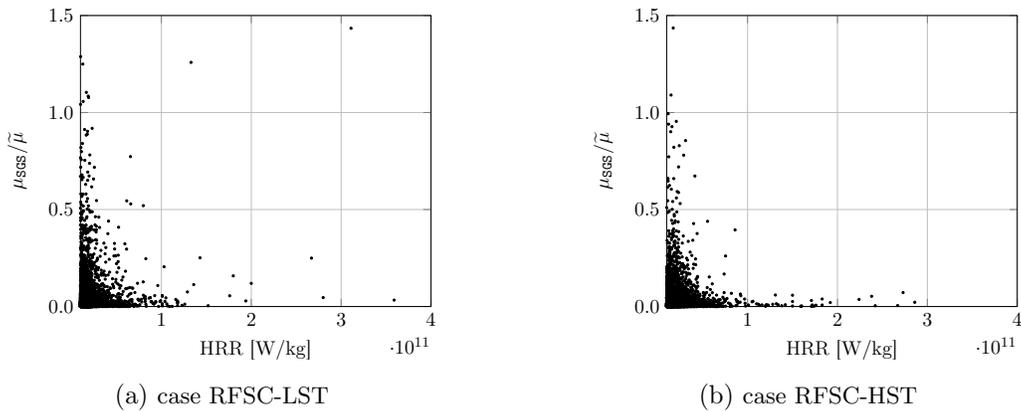


Figure 19: Scatter plot of $\mu_{scs}/\tilde{\mu}$ versus heat release rate for (a) case RFSC-LST and (b) case RFSC-HST

554 At this level, it is noteworthy that the two figures discussed above, i.e., Figs. 17 and 18,
 555 reflects the quality of the computational resolution with respect to chemical processes rele-
 556 vant to auto-ignition and flame propagation. This is confirmed by Figs. 19 which reports the
 557 viscosity ratio $\mu_{\text{SGS}}/\tilde{\mu}$ plotted versus the heat release rate (HRR). Figure 19 clearly shows that
 558 the most important part of the HRR takes place in well-resolved regions that correspond to
 559 values of $\mu_{\text{SGS}}/\tilde{\mu}$ smaller than 0.5. In these two scatterplots, more than 99% of the points are
 560 indeed associated to values of $\mu_{\text{SGS}}/\tilde{\mu}$ smaller than 0.5. Added to Figs. 17 and 18, and to the
 561 previous inspection of resolution criteria reported in section 4, it brings some additional sup-
 562 port in favor of computational mesh adequacy so as to capture the dynamics of the turbulent
 563 flame.

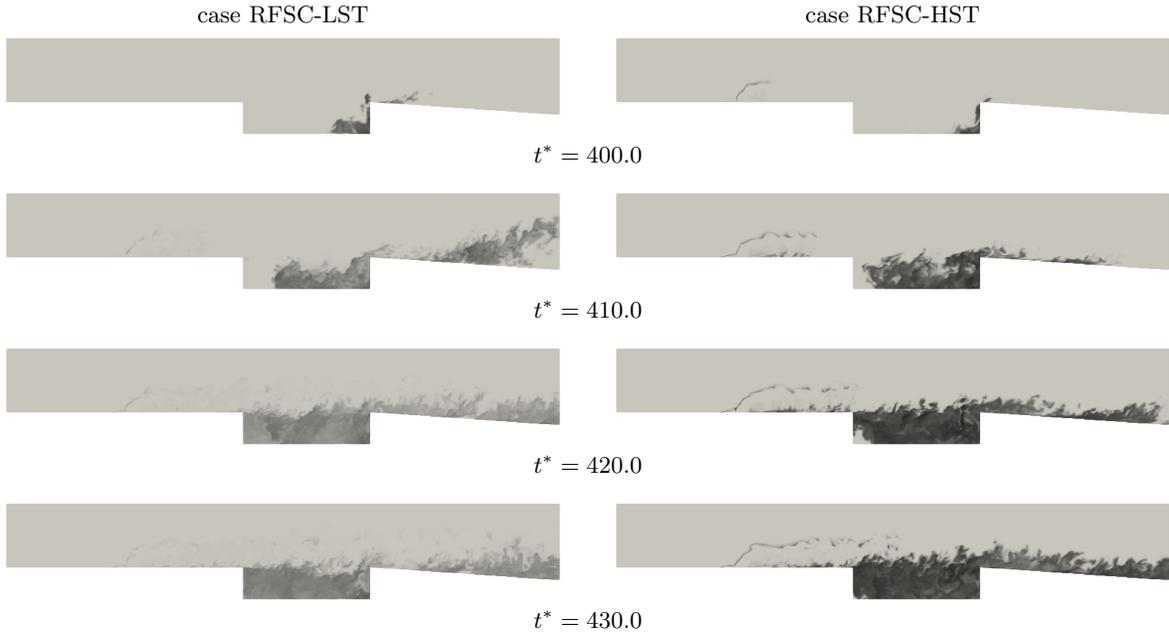


Figure 20: Temporal evolution of OH mass fraction for case RFSC-LST (left) and case RFSC-HST (right) in the median plane $x_3/D_1 = 0.0$

564 Figure 20 displays the temporal evolution of the OH mass fraction production rate in the
 565 median plane ($x_3/D_1 = 0.0$) for cases RFSC-LST and RFSC-HST. Chemical reactions start at
 566 the bottom end of the cavity for case RFSC-LST: it first develops within the cavity, increasing
 567 the temperature and inducing a deflection of the shear layer due to the thermal expansion
 568 induced by the heat release. The conditions then become more favorable to the spreading
 569 of chemical reactions as the combustion process develops, thus increasing the temperature
 570 and allowing the reaction zone to extend over the whole cavity, up to a point where the
 571 heat release rate becomes sufficient to stabilize the combustion process. Depending on the
 572 operating conditions, the combustion can spread upstream of the cavity, as it can be seen
 573 in case RFSC-HST. It is noteworthy that, as expected, the vitiated air-stream temperature
 574 significantly influences the combustion development. The combustion spreads significantly
 575 faster at a higher temperature. Significant H_2O production takes place along the upper part
 576 of the cavity for case RFSC-LST (cavity stabilized mode), whereas for case RFSC-HST (jet-

577 wake stabilized mode) combustion spreads downstream of the fuel injection and within the
 578 cavity.

579 Figure 21 reports the averaged heat release rate issued from the computations, presented
 580 in a way similar to the flame luminosity images of Micka and Driscoll (2008). To favor the
 581 comparison with the images reported in the experimental work, the HRR has been integrated
 582 along the spanwise direction. The computational results confirm that the cavity-stabilized
 583 combustion mode is characterized by a reaction zone anchored at the leading edge of the cavity,
 584 spreading into the main flow at an approximately constant angle. In the jet-wake stabilized
 585 mode the reaction zone is stabilized upstream of the cavity and the corresponding leading
 586 edge is curved. This is fully consistent with the experimental observations. Nevertheless, it
 587 should be emphasized that such a comparison remains purely qualitative since the relation that
 588 may exist between flame luminosity and HRR remains by far unknown. It is however quite
 589 interesting to see that the global change of behaviour that is observed between case RFSC-LST
 590 and case RFSC-HST is captured by the present set of computations. As underlined at the
 591 end of section 4, the mesh has been considerably coarsened downstream of the wall-mounted
 592 cavity and there are some pressure disturbances that appear at the nozzle wall. Their imprint
 593 is clearly visible on the right side of the HRR fields reported in Fig. 21.

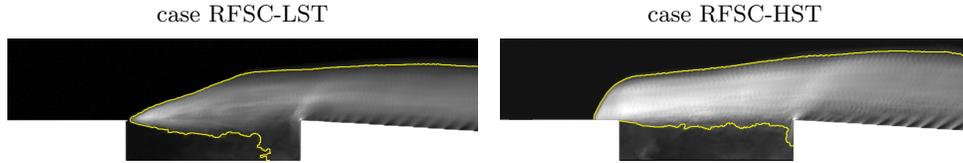


Figure 21: Averaged heat release rate (HRR) issued from the computations (arbitrary scaled units)

594 Thus, two distinct combustion stabilization modes can be inferred from the analysis of
 595 the reactive flowfield. Under moderate values of the airstream temperature (case RFSC-
 596 LST) the cavity-stabilized mode is dominant, while for larger inlet temperatures (case RFSC-
 597 HST), non-negligible water vapor dissociation and heat release occur in the vicinity of the
 598 fuel injection. These two modes are illustrated in Fig. 22, which presents an instantaneous
 599 snapshot at $t^* = 950.0$ of the iso-surface $\tilde{\xi} = 0.5$ of the filtered fuel inlet tracer $\tilde{\xi}$ (in light
 600 grey) as well as an isovalue of the OH filtered mass fraction \tilde{Y}_{OH} colored by the normalized
 601 filtered temperature \tilde{T}/T_0 , for both simulated cases.

602 Whatever the leading mechanism of combustion stabilization, e.g., self-ignition or flame
 603 propagation phenomena, the temperature of the fresh mixture T_u appears as a critical param-
 604 eter. Figure 23 presents filtered temperature scatterplots issued from the non-reactive flow
 605 simulations. It is plotted against the filtered mixture fraction $\tilde{\xi}$ together with a standard linear
 606 approximation (dashed line) and a polynomial approximation (continuous line). The linear
 607 approximation is expressed thanks to the following expression $T_u(\xi) = \tilde{\xi} T_{fuel} + (1 - \tilde{\xi}) T_{ox}$
 608 with T_{fuel} the hydrogen inlet stream temperature and T_{ox} the vitiated air inlet stream tem-
 609 perature, the values of which are provided in Table 1.

610 In fact, it must be emphasized that the use of a linear expression to express the temper-

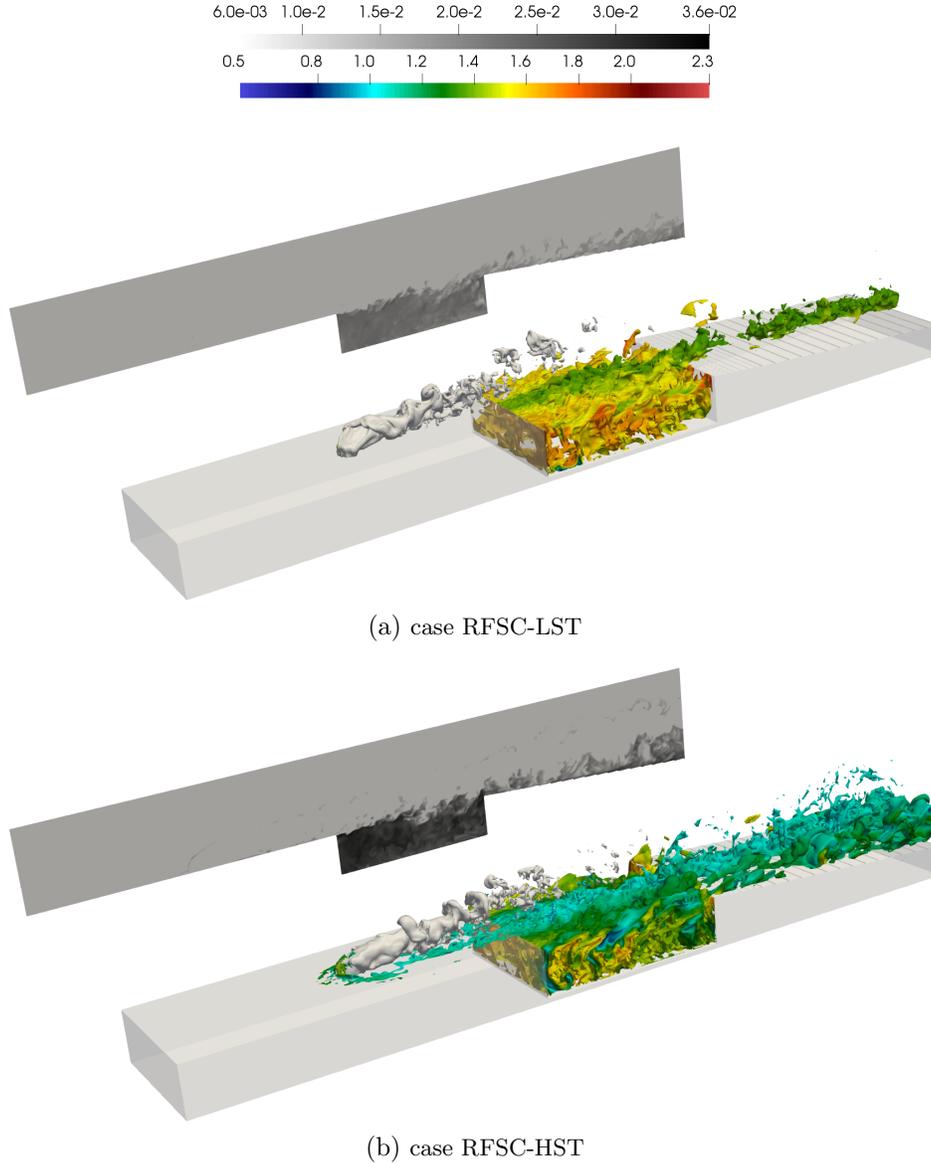


Figure 22: Isovalue surface of the OH filtered mass fraction colored by the normalized filtered temperature \tilde{T}/T_0 and fuel inlet tracer iso-surface $\tilde{\xi} = 0.5$. Back side: OH mass fraction. Top: grayscale levels associated to Y_{OH} variations, colormap associated to normalized temperature variations.

611 ature of the fresh mixture as a function of the mixture fraction is highly questionable. First,
 612 temperature is not an extensive quantity and, for such supersonic flow conditions, it would be
 613 more relevant to express the total enthalpy as a function of the mixture fraction (Mura and
 614 Iazard, 2010). As previously emphasized by Iazard et al. (2009), a linear relationship between
 615 total enthalpy and mixture fraction may hold if the Lewis and Prandtl numbers are unity and
 616 the effects induced by temporal variations of pressure remains negligible. In addition to this,
 617 it seems worth recalling that, in supersonic flow regimes, compressibility effects may play an
 618 important role, in such a manner that the linear representation may no longer be adequate
 619 because of the presence of shock and expansion waves. In the present simulation, the fuel jet

620 ($\tilde{\xi} = 1$) strongly expands, causing a significant temperature decrease. The temperature then
 621 increases with the Mach disk compression, whereas the oxidizer stream ($\tilde{\xi} = 0$) characteris-
 622 tics are altered through the bow shock compression and wall friction. Considering all these
 623 complex effects, which are difficult to include within a simple mathematical expression, it is
 624 proposed instead to fit the results of the non-reactive numerical simulation using a fourth-
 625 order polynomial approximation so as to express the temperature as a function of the mixture
 626 fraction. The corresponding evolution $T_u(\xi)$ is depicted in Fig. 23.

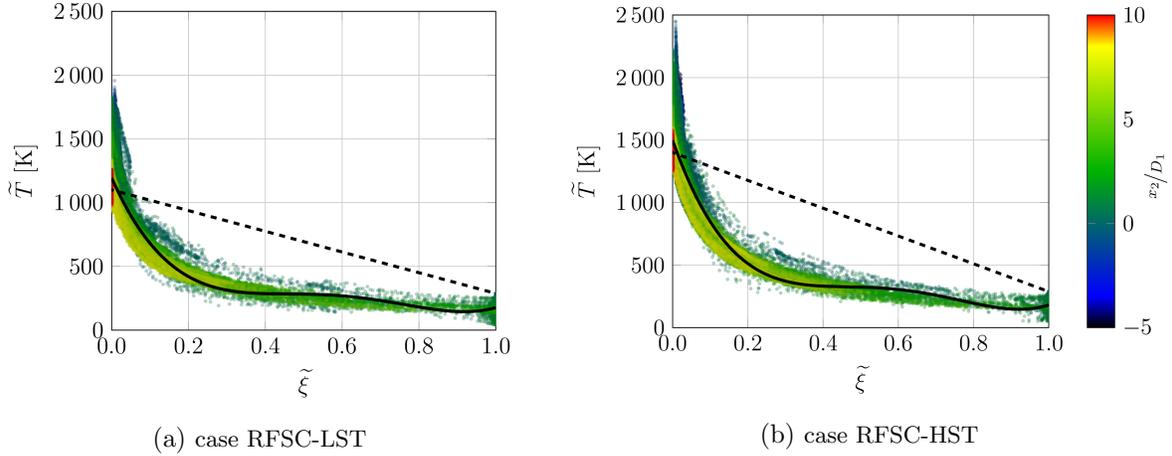


Figure 23: Scatterplots of the fresh reactant temperature

627 Since chemical reactions take place far downstream of the fuel injection, it seems worth-
 628 while to attempt to discriminate between premixed and non-premixed (i.e. diffusive) combus-
 629 tion contributions. A premixedness index $\check{\zeta}_p$ is therefore considered. It is defined as follows:

$$630 \quad \check{\zeta}_p = \frac{1}{2} (1 + \mathbf{n}_F \cdot \mathbf{n}_O) \quad (19)$$

631 with \mathbf{n}_F and \mathbf{n}_O being normal unit vectors associated to the direction of the molecu-
 632 lar diffusion fluxes of the fuel and oxidizer, respectively, which are evaluated from $\mathbf{n}_F = \tilde{\mathbf{V}}_F / \|\tilde{\mathbf{V}}_F\|$
 633 and $\mathbf{n}_O = \tilde{\mathbf{V}}_O / \|\tilde{\mathbf{V}}_O\|$ where $\tilde{\mathbf{V}}_F$ and $\tilde{\mathbf{V}}_O$ denote the filtered diffusion velocity of the fuel and
 634 oxidizer, respectively. As it is defined, this index is expected to approach zero for diffusive
 635 combustion and unity for premixed combustion. It should be fairly recognized that its repre-
 636 sentativity can be questioned in certain situations but it remains widely used in preliminary
 637 inspections of partially-premixed combustion (Martínez-Ferrer et al., 2017b). Figure 24 dis-
 638 plays the PDF of this premixedness index obtained in a volume restricted to $0.01 \leq \tilde{\xi} \leq 0.99$
 639 at several times for cases RFSC-LST and RFSC-HST⁴. The peak associated to a premixed-
 640 ness index equal to zero is much higher than the peak associated to unity indicating mostly
 641 diffusive combustion. However, the contribution of the premixed mode to the HRR is more
 642 significant and corresponds to a premixed flame structure (in red) that develops in the vicinity
 643 of the cavity leading edge, as it can be seen in the top part of Fig. 24.

⁴Only the samples associated to non-negligible values of the HRR are considered

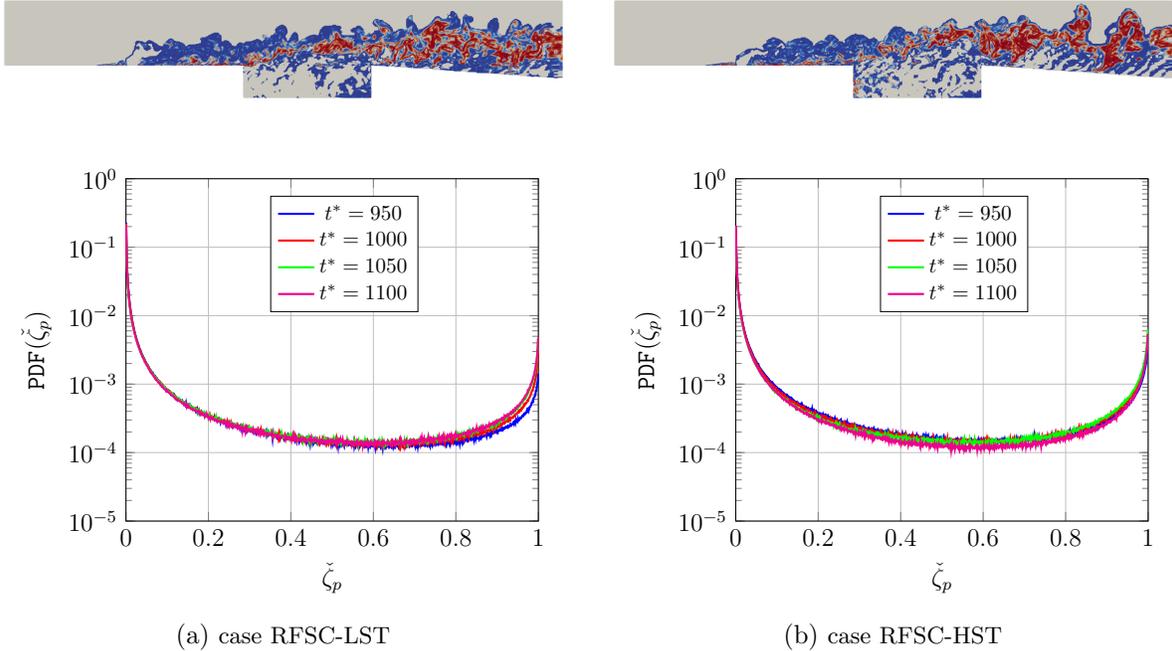


Figure 24: Premixedness index distribution: field in the median plane at time $t^* = 1100.0$ (top) and associated PDF at various times (bottom)

644 Since a non-negligible amount of chemical reaction takes place in a premixed combustion
 645 mode, attention is now focused on this contribution. To this purpose, some preliminary
 646 computations are performed with the **Cantera** software, considering mixtures of fresh reac-
 647 tants at various composition with the temperature of the fresh mixture set according to the
 648 polynomial expression $T_u(\xi)$ discussed above. The chemistry description used to perform this
 649 set of computations is the same as the one retained to perform the whole set of simulations.
 650 Figure 25 displays the self-ignition delay of the corresponding mixtures as a function of the
 651 mixture fraction (top) or equivalence ratio (bottom) for cases RFSC-LST and RFSC-HST. It
 652 is plotted together with the polynomial expression retained for the fresh reactant temperature.

653 From the obtained results, it is noteworthy that, as the mixture fraction is increased from
 654 the left to the right side of Fig. 25, the self-ignition delay first decreases and displays a local
 655 minimum for the most reactive conditions ξ_{mr} and then increases, until it reaches very large
 656 values for rich mixtures. As expected, the most reactive state, which corresponds to a minimal
 657 value of the self-ignition delay, does not correspond to stoichiometry. This is a direct outcome
 658 of the vitiation of the oxidizer inlet stream, which features a temperature that is significantly
 659 larger than the one of the fuel inlet stream. It is also remarkable that the self-ignition delay
 660 displays a sharp increase for rich conditions, in such a manner that spontaneous ignition
 661 regimes are less likely for these mixtures. More precisely, the corresponding auto-ignition
 662 regimes require more time to develop, which may favor premixed flame propagation. We will
 663 see below that the characteristic time scales of premixed flame propagation indeed remain
 664 significantly smaller than the ignition delays for such rich mixtures. However, as long as lean
 665 conditions are considered, only the auto-ignition regimes are expected to occur.

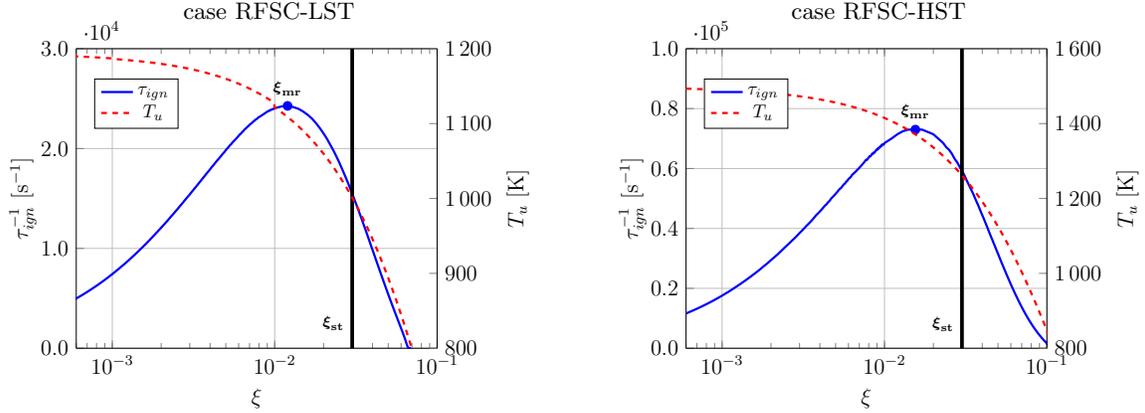


Figure 25: Self-ignition delay τ_{ign} as a function of the mixture fraction

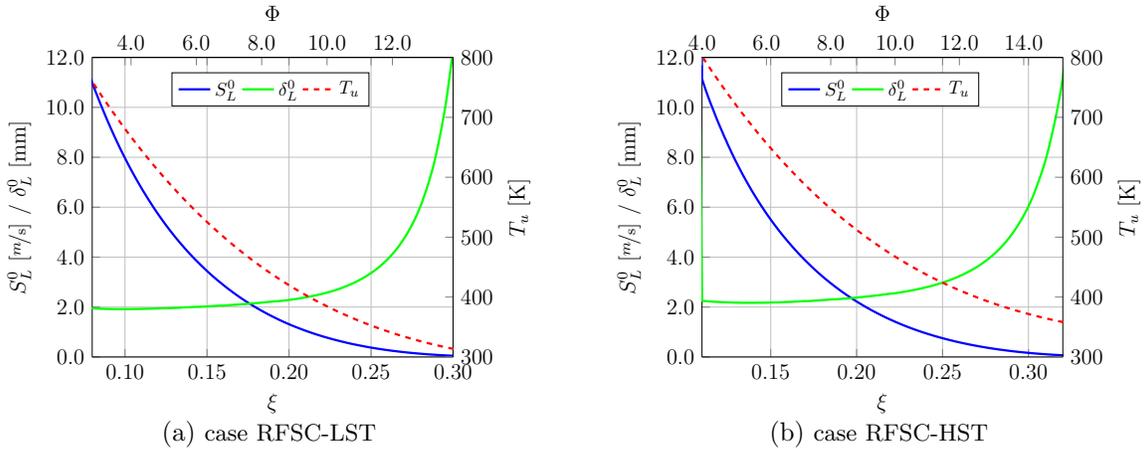


Figure 26: Laminar flame velocity S_L^0 and thickness δ_L^0 as functions of the mixture fraction

666 Figure 26 displays the evolution of the laminar premixed flame velocity S_L^0 and associated
667 flame thickness δ_L^0 computed again with the detailed chemical mechanism of O’Conaire et al.
668 (2004). In this figure, for both conditions (RFSC-LST and RFSC-HST), the left boundary of
669 the depicted mixture fraction range corresponds to the value below which flame propagation
670 is no longer relevant. Indeed, below this value, it becomes impossible to perform the premixed
671 flame computation because self-ignition may occur. For such values of the mixture fraction,
672 the computations thus displays an exacerbated sensitivity to numerical simulation parameters
673 including the length of the computational domain, the number of computational nodes, the
674 choice of the integration time step, etc. This is in contrast to the right boundary of the
675 mixture fraction domain beyond which the laminar flame propagation velocity tends to zero;
676 it corresponds to the high flammability limit. In this respect, the figure shows that, as S_L^0
677 decreases, the flame thickness δ_L^0 increases also, up to the flammability limit. The associated
678 flame propagation time scale or flame transit time, defined as $\tau_L^0 = \delta_L^0/S_L^0$, is displayed as a
679 function of the mixture fraction in Fig. 27. In a restricted mixture fraction domain bounded
680 by the two limits discussed above, the laminar premixed flame velocity S_L^0 (resp. the transit
681 time scale τ_L^0) decreases (resp. increases) with the mixture fraction, as it is shown in Figs. 26

682 and 27. The laminar premixed flame velocity should reach a maximum in the vicinity of
 683 the stoichiometry but, as emphasized above, the self-ignition mechanism is the leading order
 684 phenomnom for these compositions of the reactive mixture.

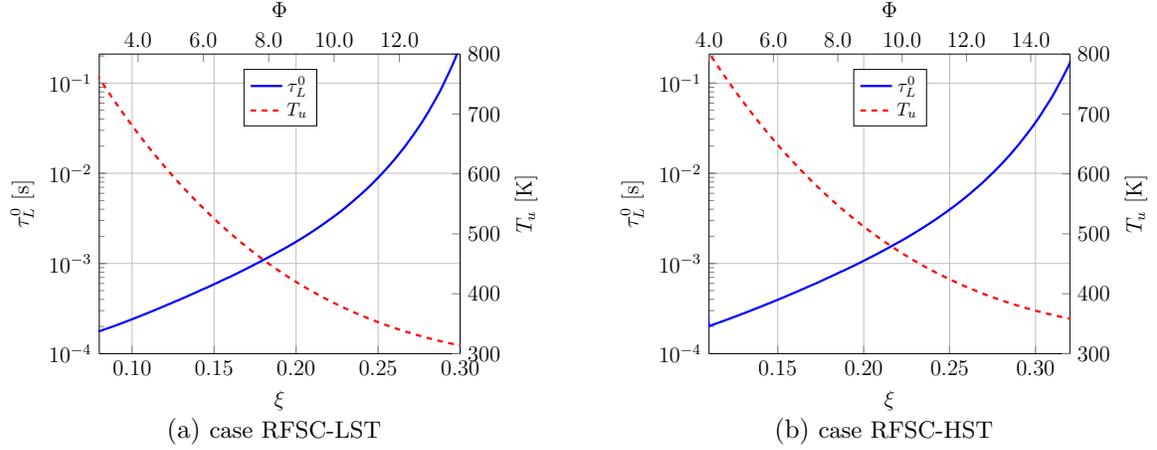


Figure 27: Flame propagation timescale τ_L^0 as a function of the mixture fraction

685 Turbulent premixed combustion regimes are now analyzed using the coordinates intro-
 686 duced by Barrère and Borghi (Borghi, 1984, 1985). The data are thus plotted in Fig. 28 using
 687 a normalized length scale ratio ℓ_t/δ_L^0 and velocity ratio u_{rms}/S_L^0 as the set of coordinates. In
 688 these expressions, the turbulence integral length scale is approximated from $\ell_t = u_{rms}^3/\varepsilon$ with
 689 ε the resolved molecular dissipation rate, which has been evaluated as the trace of the second
 690 rank resolved molecular dissipation rate tensor, i.e.,

$$\varepsilon_{ij} = \frac{1}{\langle \rho \rangle} \left\langle \left(\bar{\tau}_{ik} - \langle \bar{\tau}_{ik} \rangle \right) \frac{\partial}{\partial x_k} \left(\frac{\bar{\rho} \tilde{u}_j - \langle \bar{\rho} \tilde{u}_j \rangle}{\langle \rho \rangle} \right) + \left(\bar{\tau}_{jk} - \langle \bar{\tau}_{jk} \rangle \right) \frac{\partial}{\partial x_k} \left(\frac{\bar{\rho} \tilde{u}_i - \langle \bar{\rho} \tilde{u}_i \rangle}{\langle \rho \rangle} \right) \right\rangle \quad (20)$$

691 The velocity fluctuation RMS is approximated from $u_{rms} = \sqrt{2k/3}$ with k the resolved
 692 turbulent kinetic energy, which is evaluated from $k = (\langle \bar{\rho} \tilde{u}_i \tilde{u}_i \rangle - \langle \bar{\rho} \rangle \langle \tilde{u}_i \rangle \langle \tilde{u}_i \rangle) / (2 \langle \bar{\rho} \rangle)$. The
 693 flame characteristics are estimated from the local conditions associated to the corresponding
 694 unburnt mixtures. Quantities S_L^0 and δ_L^0 are thus computed at each computational point that
 695 fulfills the following two conditions: (i) the mixture fraction remains within the lean and rich
 696 flammability limits, i.e., within a range where premixed flame propagation may occur, and
 697 (ii) the considered point lies inside a zone where the probability to obtain a premixed flame
 698 structure remains larger than a given threshold value, which is presently set to 40%.

699 Figure 28 shows that, from one location to another, the turbulent combustion regimes
 700 are highly variable. Some points correspond to quasi-laminar conditions, while others feature
 701 strong turbulence-chemistry interactions (TCI). It should be emphasized that, with thick
 702 flames, thickened-wrinkled flames, and even laminar ones, almost all possible turbulent com-
 703 bustion regimes may be found. In condition RFSC-LST, most of the points are located in
 704 the vicinity of thickened-wrinkled flame regime, between the line $Da = 1.0$ and the Klimov-

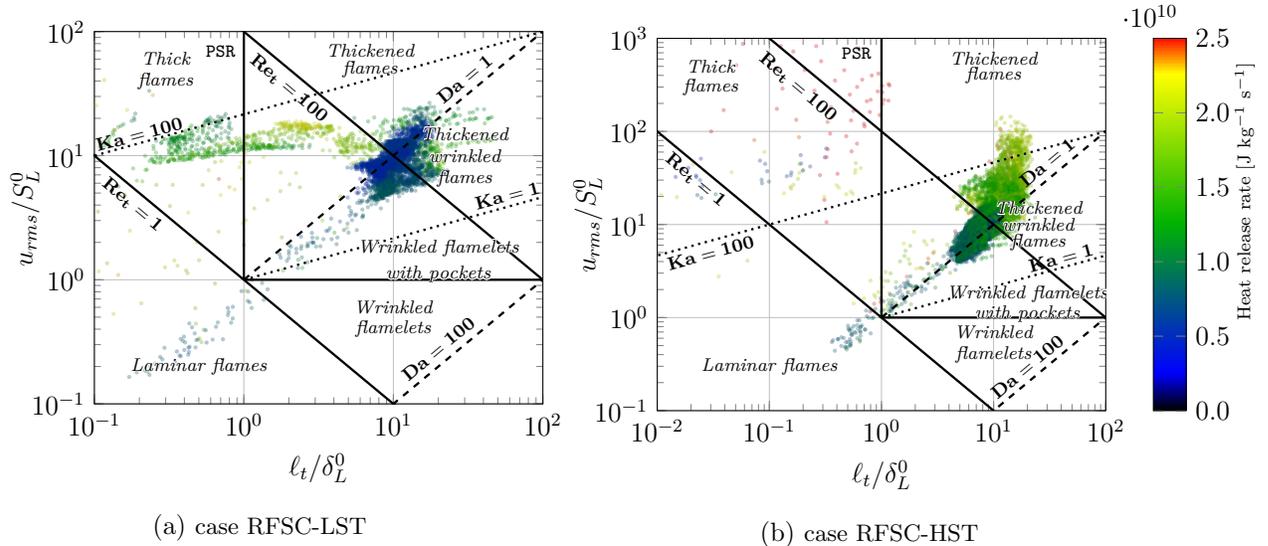


Figure 28: Premixed turbulent combustion diagram based on the Borghi-Barrère coordinates (Borghi, 1985)

705 Williams limit⁵ (Williams, 1976), around the horizontal line corresponding to $u_{rms}/S_L^0 = 10.0$.
 706 These regimes are consistent with those previously reported by Quinlan et al. (2014) for scram-
 707 jet conditions. There are also some points featuring a non-negligible heat release rate located
 708 in the thick flame region. It is noteworthy that the corresponding points are located in the
 709 vicinity of the hydrogen injection, where the reactive mixture remains highly segregated and
 710 velocity fluctuations are quite large. On average, the case RFSC-HST displays significantly
 711 larger heat release rates, with a statistics spread towards the thickened and thickened-wrinkled
 712 flame regimes, which corresponds to smaller values of the Damköhler number. Also, chemical
 713 reactions take place at locations where velocity fluctuations may reach extremely large values
 714 and, as a consequence, non-negligible finite-rate chemistry effects come into play.

715 It is noteworthy that the above evaluation of the dissipation rate ε does not account for
 716 the unresolved (i.e., modelled) contribution. The relevance of this approximation can be
 717 evaluated through a complementary analysis of the computational results. The objective of
 718 this analysis is to provide an additional assessment of the LES resolution level by investigating
 719 the contribution of the SGS model to the turbulent energy dissipation. To quantify the SGS
 720 contribution, one can define two components $\varepsilon_{(SGS)}$ and ε'_{SGS} , which are acting on the resolved
 721 turbulent kinetic energy and SGS turbulent kinetic energy $\langle k_{SGS} \rangle$, see for instance Ben-Nasr
 722 et al. (2017). Following Davidson (2006), these two components can be formulated in such a
 723 manner that

$$\varepsilon_{SGS} = \varepsilon_{(SGS)} + \varepsilon'_{SGS} \quad (21)$$

724 where the two contributions are evaluated from

$$\varepsilon_{(SGS)} = \frac{1}{\langle \rho \rangle} \langle T_{ij}^* \rangle \frac{\partial \langle \tilde{u}_j \rangle}{\partial x_k} \quad (22)$$

⁵It may be worthwhile to recall that this limit corresponds to $Ka = 1.0$.

725 and

$$\varepsilon'_{\text{SGS}} = \frac{1}{\langle \rho \rangle} \left\langle \left(T_{ij}^* - \langle T_{ij}^* \rangle \right) \frac{\partial}{\partial x_k} \left(\frac{\overline{\rho u_j} - \langle \overline{\rho u_j} \rangle}{\langle \rho \rangle} \right) \right\rangle \quad (23)$$

726 with T_{ij}^* the deviatoric part of the subgrid-scale (SGS) stress tensor T_{ij} .

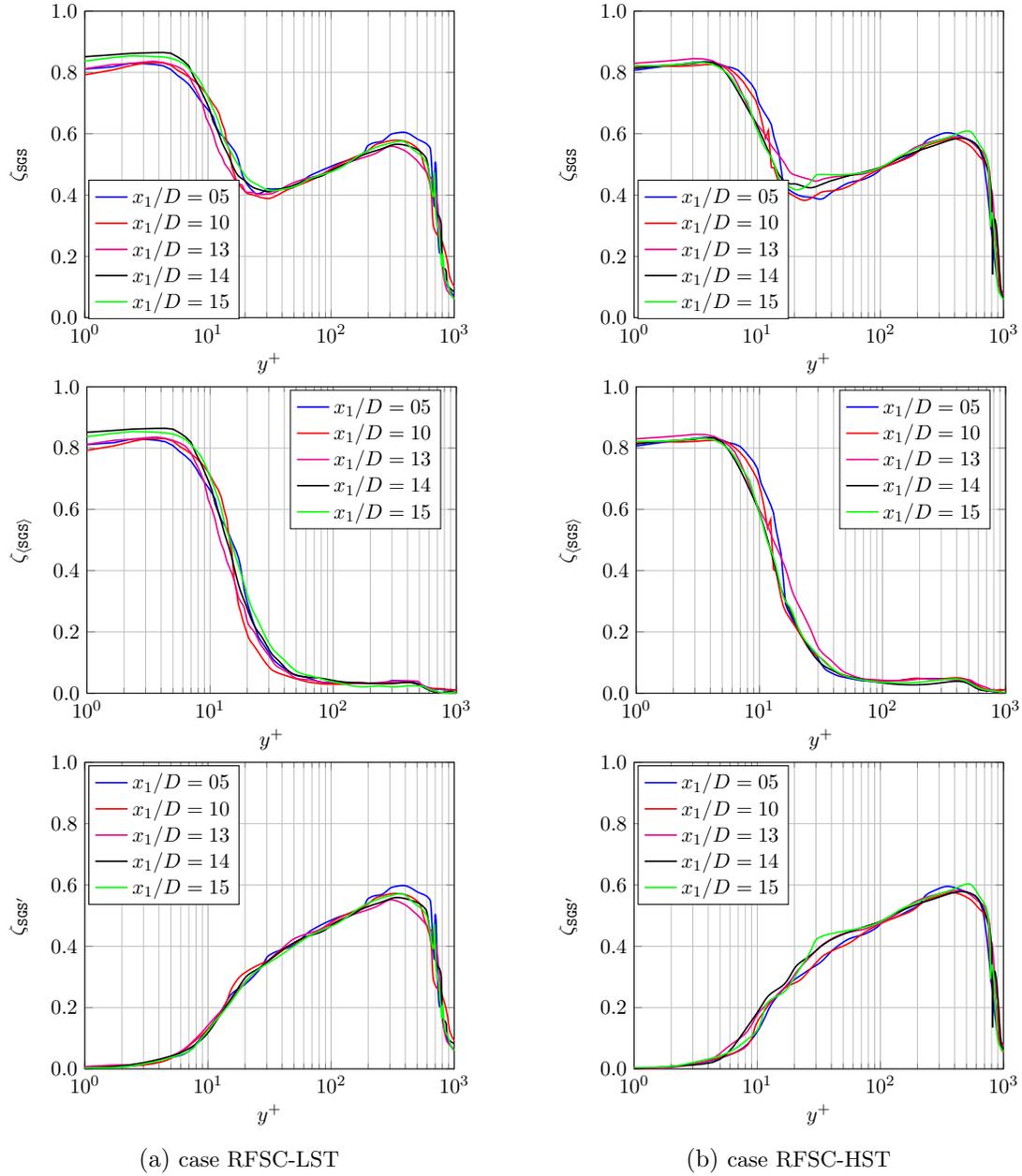


Figure 29: SGS Activity parameters as functions of y^+

727 As defined above, the total SGS dissipation of a LES model, ε_{SGS} , is the sum of both the
 728 SGS dissipation associated to the average of the filtered flowfield, $\varepsilon_{\langle \text{SGS} \rangle}$, and the one due to
 729 the fluctuating flowfield, $\varepsilon'_{\text{SGS}}$. Thus, a global SGS activity parameter can be defined as:

$$\zeta_{\text{SGS}} = \frac{\varepsilon_{\text{SGS}}}{\varepsilon_{\text{SGS}} + \varepsilon} \quad (24)$$

730 while the activities due to the averaged and fluctuating flowfield can be discriminated by
 731 considering instead

$$\zeta_{\langle \text{SGS} \rangle} = \frac{\varepsilon_{\langle \text{SGS} \rangle}}{\varepsilon_{\langle \text{SGS} \rangle} + \varepsilon} \quad (25)$$

732 and

$$\zeta'_{\text{SGS}} = \frac{\varepsilon'_{\text{SGS}}}{\varepsilon'_{\text{SGS}} + \varepsilon} \quad (26)$$

733 These three indexes are reported in Fig. 29. This figure displays the SGS activity pa-
 734 rameter ζ_{SGS} , together with its two components $\zeta_{\langle \text{SGS} \rangle}$ and ζ'_{SGS} , as functions of y^+ at different
 735 cross-stream locations. In the viscous sublayer and up to $y^+ = 5$, the value of the SGS activity
 736 parameter ζ_{SGS} (top of Fig. 29) is approximately equal to 0.8. In the transition region and
 737 up to $y^+ = 300$, it decreases and reaches a minimum of 0.4 at $y^+ = 20$, ζ_{SGS} increases in the
 738 outer region of the boundary layer and reaches a maximum value of about 0.6, to decrease
 739 again at the edge of the boundary layer. The SGS activity parameter $\zeta_{\langle \text{SGS} \rangle}$ associated to
 740 the filtered-averaged flowfield (middle of Fig. 29) confirms that the SGS dissipation is mainly
 741 driven by viscous effects in the near-wall region, while the fluctuating velocity field is domi-
 742 nant in the transition and outer regions. Not only the behaviour but also the values reported
 743 above are fully consistent with the results previously obtained with the WALE subgrid-scale
 744 closure by Ben-Nasr et al. (2017).

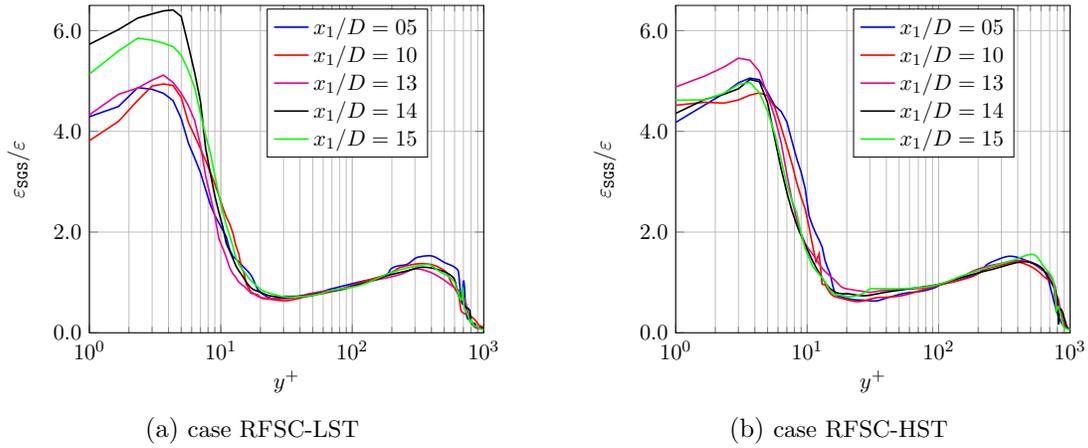


Figure 30: Ratio of the SGS dissipation to the viscous dissipation, i.e., $\varepsilon_{\text{SGS}}/\varepsilon$, as a function of y^+

745 Finally, the ratio of the SGS dissipation ε_{SGS} to the resolved viscous dissipation ε_{SGS} is
 746 plotted as a function of y^+ in Fig. 30. It is remarkable that, in a wide range of the boundary
 747 layer, from about $y^+ = 15$ to $y^+ = 200$, this ratio takes values smaller than unity and, even at
 748 larger distances from the wall, it does exceed 1.5. This confirms that the resolved dissipation
 749 rate ε , as given by Eq. 20, provides a rather satisfactory estimate of the TKE dissipation
 750 rate, which can be used to evaluate characteristic turbulence scales so as to proceed with a
 751 qualitative inspection of turbulent combustion regimes.

752 **6. Summary and conclusions**

753 A new set of highly-resolved large-eddy simulations is presented. It corresponds to the
754 geometry of a jet in a supersonic crossflow (JISCF) of vitiated air delivering hydrogen up-
755 stream of a squared cavity. The conditions are relevant to experiments previously conducted
756 at the University of Michigan. To the best of the authors' knowledge, this is the first detailed
757 computational investigation of this experimental test case. The computations are performed
758 with the computational solver **CREAMS** and make use of a recent immersed boundary method
759 (**IBM**) algorithm. The wall-adapting local eddy (**WALE**) model is retained as the subgrid-scale
760 viscosity closure. Several criteria are used to check the computational resolution, especially
761 near the walls, which are represented through an **IBM**, where some efforts have been spent
762 to capture the flow as accurately as possible. The use of the **WALE** model allows to sat-
763 isfactorily recover the behavior in the buffer layer that separates the logarithmic zone from
764 the viscous sublayer. The filtered chemical rates are represented using either the **PSR** or the
765 **U-PaSR** closures and it is remarkable that, for the present level of computational resolution,
766 the results obtained using the two distinct frameworks are very similar.

767 Depending on the inlet vitiated airstream temperature, two stabilization modes are re-
768 covered: cavity-stabilized regime and jet-wake stabilized regime. In the cavity-stabilized
769 combustion mode, combustion is anchored at the leading edge of the wall-mounted cavity and
770 spreads into the main flow at an approximately constant angle, whereas jet-wake stabilized
771 combustion takes place directly downstream of the fuel injection, i.e., upstream of the cavity.
772 In this respect, it seems worth mentioning that different averaged streamline flowfields – not
773 reported for the sake of conciseness – have been obtained for cavity and jet-wake stabilization
774 modes. For high operative temperatures, combustion primarily takes place in the jet-wake
775 stabilization mode while, for lower operative temperatures, the cavity stabilization mode is
776 obtained. This is consistent with the experimental results of Micka and Driscoll (2008). In
777 this respect, the present set of computations constructively complements the experimental
778 data, e.g., the corresponding computational data are used to discriminate the contributions
779 of premixed and non-premixed combustion modes. The turbulent combustion regimes are
780 also inspected on the basis of classical combustion diagrams for the two levels of inlet temper-
781 ature that have been considered. This analysis confirms the occurrence of highly turbulent
782 premixed flame conditions. For intermediate values of the operative temperature, some oscil-
783 lations between the two modes are expected and it would be interesting to run complementary
784 numerical simulations at these intermediate operative temperatures so as to understand how
785 these oscillations may happen and how long each stabilization mode is active. This offers an
786 interesting perspective for future works.

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