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Analysis of high-speed combustion regimes of hydrogen jet in supersonic vitiated airstream

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Abstract

Highly-resolved reactive simulations of a hydrogen jet injected into a transverse supersonic flow of vitiated air at Mach 2 are conducted. The operating conditions are chosen to be relevant of scramjet operative conditions and are representative of experiments conducted at ONERA Palaiseau Research Center. Hydrogen injection in the supersonic vitiated airstream leads to the formation of a bow shock, which interacts with the boundary layer and gives rise to separation zones. In the resulting recirculation zones, only small amounts of OH radicals are produced. Combustion stabilization and development take place further downstream. Heat release is significant in the vicinity of the wall within a sonic region where the equivalence ratio is around two. Farther from walls, combustion takes place at supersonic speeds but features lower levels of heat release rates. Supersonic turbulent combustion regimes are analyzed in detail: first in a standard set of coordinates $(u'/S_L^0, L_t/\delta_L^0)$ using data collected in regions featuring a sufficiently large degree of premixing. Then, they are analyzed in the turbulent Reynolds and Damköhler numbers sub-space (Re_t , Da). In this representation, three distinct Damköhler number definitions based on (i) production rate of H₂O. (*ii*) flame propagation characteristic time, and (*iii*) ignition delay time are considered. These various representations put into evidence turbulent combustion regimes featuring significant finite-rate chemical kinetics effects. The whole set of computational results confirms that (i) the use of models based on the fast chemistry hypothesis is questionable for such conditions, *(ii)* taking into account finite-rate chemistry effects is essential, and (iii) ignition processes play a key role in combustion stabilization. The manuscript ends with some perspectives and challenging issues for future works.

Keywords: high-speed flows, supersonic combustion regimes, jet in

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supersonic crossflow, turbulent combustion, finite-rate chemistry, hydrogen combustion

1 1. General introduction

The contribution of K. N. C. Bray to combustion science has laid the foundations for the turbulent premixed flame theory [1-23]. Indeed, his outstanding input into the mathematical description of turbulent premixed flames in the thin flame limit [1-8] has provided a solid and seminal basis for most of the fundamental research studies conducted in the field [24-33] and it remains today's cornestone of current research works devoted to the analysis and modelling of turbulent premixed combustion [34-41].

Thus K.N.C. Bray has been one amongst the pioneers in the use of sta-9 tistical approaches to describe turbulent reacting flows. From the combined 10 use of probability density functions (PDF), intermittency theory, and asymp-11 totics [6], the fundamental and underlying physical mechanisms were identi-12 fied. A typical (and remarkable) example is provided by Bray's early deriva-13 tion of the relationship between the mean chemical rate and mean scalar dis-14 sipation rate (SDR) of reactive species [4], a quantity that is indeed central to 15 a wide range of turbulent combustion closures for premixed and partially pre-16 mixed conditions, e.g., [29, 42–50]. Complete sets of second-order turbulence 17 models have been also proposed so as to take the influence of thermal ex-18 pansion into account. Their early developments lead to (i) the identification 19 of the so-called flame-generated turbulence (FGT) production and counter-20 gradient diffusion (CGD) or non-gradient diffusion phenomena [7, 8] and *(ii)* 21 the detailed analyses of the role played by pressure terms, *i.e.*, correlations 22 between the pressure fluctuations and velocity (or composition) gradients, 23 under the influence of local flamelet contributions [21]. With all these de-24 velopments and seminal findings, K.N.C. Bray has provided solid bases for 25 the development of flamelet methods, which offer a robust framework for the 26 modelling of turbulent combustion [11]. 27

In fact the contribution of K.N.C. Bray to turbulent premixed combustion is so significant that this has somehow hidden some of his other pieces of work in the field of chemical physics, ionized multicomponent mixtures and plasmas, gas dynamics, and high-speed flows in general [51–57].

From a general viewpoint, combustion in high-speed (supersonic) flows is relevant to security and safety issues, atmospheric re-entry flows, astrophysics [58], hypersonic propulsion systems [59], rocket engines and igniters, such as the one considered in reference [60]. As regards its appli-

cation to propulsion, one of the most typical examples is the scramjet en-36 gine [59, 61, 62]. For flight Mach number values larger than five (hypersonic 37 flight), attention has been indeed early focused in the late fifties on the 38 possibility of performing the combustion at supersonic speed so as to avoid 39 the prejudicial effects of dissociation on combustion efficiency. Supersonic 40 combustion was proven to be possible as early as 1962 at the Aerodynamics 41 Laboratory of the Polytechnics Institute of Brooklyn (PIBAL) where, almost 42 50 years ago, combustion was stabilized in the supersonic coflowing streams 43 geometry, see Ferri, Libby, and Sakkay [63]. 44

In this respect, the early contribution of K.N.C. Bray to combustion 45 in high-speed flow conditions — a challenging combustion regime that, for 46 many years, has concentrated significant research efforts — has settled some 47 of the bases of turbulent reactive flow modelling in these extreme condi-48 tions. The description of turbulent combustion in supersonic flows has been 49 central to a reference book chapter written by K.N.C. Bray, P.A. Libby, 50 and F.A. Williams [64]. The topic has been also covered by P.A. Libby in 51 reference [65]. 52

In comparison with their low-speed counterparts, reactive high-speed 53 flows indeed raise some specific issues. For instance, these reactive high-54 speed flows do involve some special couplings between chemical reactions and 55 compressibility effects, *i.e.*, compression waves and rarefaction waves. This 56 is because the gas temperature is sensitive to these compression/rarefaction 57 waves. Thus, there is a permanent exchange between internal energy (molec-58 ular scale) and kinetic energy (macroscopic scale). In this respect, it does 59 not seem useless to remind here that the Mach number Ma is the squared 60 root of the ratio between the kinetic energy (of the flow) and thermal energy 61 or static enthalpy, *i.e.*, the average kinetic energy of molecules. In the vicin-62 ity of sonic conditions (Ma = 1), the kinetic energy is indeed already of the 63 same order of magnitude as the static enthalpy per unit mass and it becomes 64 the main contribution as the Mach number value is increased beyond unity. 65 Therefore, since the kinetic energy dissipation induced by molecular viscos-66 ity effects, in boundary layers, shear layers or shock waves, is proportional 67 to the squared Mach number Ma², moderate changes in velocity result in 68 non-negligible changes in static temperature and pressure. Considering the 69 sensitivity of chemical reactions to temperature and pressure, this induces a 70 coupling between the velocity field and chemical reactions. The considera-71 tion of these effects therefore appears as one amongst the specific challenges 72 of high-speed turbulent combustion modelling and the early works of Bray 73 and his coworkers [66, 67] has served as a basis to some of the seldom mod-74 elling proposals that attempted to address this issue [68-72]. In this respect, 75

the early developments made in references [66–68] were conducted within
the laminar flamelet framework and this raises the question of the combustion regimes [73, 74] relevant to such conditions. This specific — and still
open question — that has seldom been addressed [75–77] since the work of
Balakrishnan and Williams [75] is central to the present study.

The manuscript is organized as follows: the next section (Sec. 2) provides a brief overview of the computational database that is used to proceed with the present investigation; it is followed by a short section (Sec. 3) where some features of the unburnt mixture (temperature and reactivity) are scrutinized. The analysis of high-speed combustion regimes, which is the core of the present study, is detailed in Sec. 4. Finally, perspectives for future works are gathered in a conclusion section that ends the manuscript.

Table 1: Main characteristics of the computational grid. The lengths and mesh sizes are normalized by D, the diameter of the injector.

| direction | x | y | z |
|----------------------------|----------------|------------------|----------------|
| length | 190.0 | 8.85 | 20.0 |
| number of points N_{x_i} | 2253 | 196 | 193 |
| stretching factor $(\%)$ | 0.35 to 0.55 | 2.0 to 3.0 | 1.70 to 3.15 |
| mesh sizes | 0.03 to 0.10 | 0.003 to 0.250 | 0.03 to 0.30 |

2. Overview of the computational setup and database

The present analysis is based on highly-resolved numerical simulations 89 databases obtained with the massively parallel solver CREAMS. It solves the 90 three-dimensional unsteady compressible Navier–Stokes equations for multi-91 component reactive mixtures by combining high-order spatial discretization 92 schemes (7th order WENO and 8th order centered) with a 3rd order time 93 integration. Its capabilities have been previously assessed through many 94 computational investigations devoted to high-speed flows [60, 72, 78–87]. 95 The details of the mathematical model and numerical methods used in the 96 solver are not reported here, just for the sake of conciseness, and can be 97 found together with an extensive verification and validation of the compu-98 tational solver in references [88, 89]. The set of transport equations that 99 has been solved can be found in reference [81]. Finally, it must be precised 100 that the present computation has been conducted using a modified version 101 of the Hirschfelder and Curtiss approximation to evaluate mass diffusion 102 coefficients [90]. 103

| | hydrogen jet | vitiated airstream |
|---|-------------------------|----------------------|
| ξ (-) | 1.0 | 0.0 |
| $Y_{{ m H}_2}$ (-) | 1.0 | 0.0 |
| $Y_{\rm O_2}$ (-) | 0.0 | 0.2527 |
| $Y_{\rm H_2O}$ (-) | 0.0 | 0.1631 |
| $Y_{\rm N_{2}}$ (-) | 0.0 | 0.5842 |
| $p \ / \ p_0 \ ({ m Pa} \ / \ { m Pa})$ | $502,918 \ / \ 958,055$ | $56000 \ / \ 409000$ |
| $T \ / \ T_0 \ ({ m K} \ / \ { m K})$ | $248\ /\ 300$ | $1108 \ / \ 1695$ |
| $ ho~({\rm kg}{\cdot}{ m m}^{-3})$ | 0.490 | 0.161 |
| γ (-) | 1.42 | 1.27 |
| Ma (-) | 1.0 | 2.0 |
| $u \; (\mathrm{m} \cdot \mathrm{s}^{-1})$ | 1204 | 1313 |
| $m (g \cdot s^{-1})$ | 1.85 | 146.55 |

Table 2: Hydrogen jet and vitiated air inlet boundary conditions [91].

The configuration corresponds to the three-dimensional simulation of a 104 sonic hydrogen jet issuing from a flat plate into a Mach 2 vitiated air cross-105 flow. Such a geometry is well-known and often referred to as a jet in super-106 sonic crossflow (JISCF). It is sketched in Fig. 1. The conditions are represen-107 tative of those considered in the dual mode ramjet investigations conducted 108 on the LAPCAT-II setup in the ONERA-LAERTE facility [91–93]. In the 109 present study, the computational domain is reduced to a restricted part of 110 the experimental setup: it corresponds to the full width and half-height of 111 the real combustion chamber and the computation meets the inlets flow con-112 ditions (*i.e.*, those associated to the hydrogen and vitiated air streams) in 113 terms of velocity, pressure, composition, and temperature. Since the com-114 puted geometry is only half of the height of the real geometry and since an 115 extrapolation boundary condition (BC) is specified at the top of the com-116 putational domain¹, there is no possible shock wave reflection, which is a 117 significant difference between the retained computational geometry and the 118 real LAPCAT-II combustor. In addition to this, it is noteworthy that some 119 computations of the LAPCAT-II combustor model have been shown to ex-120 hibit some sensitivity to wall roughness and heat transfer modelling. One 121 may expect that the consideration of these two effects, which is outside the 122 scope of the present study, may influence the computational results. In this 123

¹Further detail about the BC specification is provided below.

regard, according to the recent study of Pelletier *et al.* [93], it may affect the location of the combustion stabilization region.

The dimensions of the corresponding domain together with the main 126 characteristics of the computational grid are reported in Table 1. The cor-127 responding cartesian grid is depicted in Fig. 2. The quantity x denotes the 128 streamwise coordinate, y is the wall-normal coordinate, and z is the span-129 wise coordinate. The quality of the computational grid has been assessed 130 by using the detailed procedure described in reference [86], which has been 131 introduced to analyze mesh reliability. The corresponding procedure com-132 bines several verification subsets including (i) the inspection of distributions 133 of wall mesh sizes, *(ii)* the analysis of normalized velocity profiles in bound-134 ary layers, and (iii) the verification of some mesh quality indexes distribu-135 tions [94, 95]. In this respect, it has been found that ninety-nine percent 136 of the computational cells feature a value of the Pope's quality index IQ_k 137 that is larger than 0.92. At this level, it seems also worth precising that 138 the present highly-resolved large-eddy simulation has been conducted with 139 the WALE sub-grid scale (SGS) viscosity model and the mesh quality has 140 been also analyzed through the inspection of viscosity ratio profiles and wall-141 normalized velocity profiles as previously reported by Techer *et al.* [81] and 142 Ribeiro et al. [86]. They are not included here just for the sake of concise-143 ness. As regard chemical reactions, no sub-grid turbulent combustion model 144 has been used, on the grounds that, in the region of interest for this study – 145 where the heat release rate (HRR) is significant — the resolved scales con-146 trol the combustion processes. Indeed, in the vicinity of the wall — where 147 combustion develops — the flow (*i.e.*, velocity) field resolution requirement 148 itself is very constraining. In this respect, SGS-based Damköhler number 149 values were evaluated from various definitions based on either the fuel con-150 sumption rate or on the overall production/destruction rates of intermediate 151 species such as hydrogen atom H or hydroperoxyl radical HO₂. Their values 152 were systematically found to be smaller than unity. Ror instance, based on 153 the hydroperoxyl radical HO_2 , more than ninety-nine percent of the values 154 obtained for $Da_{sgs} = \tau_{sgs}/\tau_{HO_2}$ are smaller than 0.1 and, according to the lit-155 erature, see for instance Bouheraoua *et al.* [96], values of Da_{sgs} smaller than 156 unity also reflects — to some extent — the quality of the computational 157 resolution. From all the information that has been gathered, it seems that 158 the present computation is indeed a highly-resolved LES that is approaching 159 DNS resolution requirements in the region where the HRR becomes signif-160 icant. As a consequence, the notation retained for any filtered quantity \tilde{q} 161 will not be discriminated from its instantaneous counterpart q. Thus, the 162 filtered value will be hereafter denoted by q just for the sake of simplicity. 163

In this respect, it is also noteworthy that the averaged value will be denoted by $\langle q \rangle$, while its Favre-averaged counterpart will be denoted by $\{q\}$.

The computational domain extends from -40.0 D upstream to 150.0 D166 downstream of the fuel injector exit along the streamwise direction, with D167 being the diameter of the injector, see Fig. 1 and Fig. 2. Along the span-168 wise and wall normal directions, the domain extends over 20.0 D and 8.85 D, 169 respectively. The sonic jet of pure hydrogen is vertically injected through 170 an orifice of diameter D = 2.0 mm. The jet exit conditions correspond to 171 a value of the jet-to-freestream momentum flux ratio $J = (\rho u^2)_{jet}/(\rho u^2)_{\infty}^2$ 172 that is approximately 2.44 and to a nozzle pressure ratio (NPR = $p_{0,iet}/p_{\infty}$) 173 approximately equal to seventeen. The boundary layer thickness is equal 174 to 1.1 D at the inlet of the computational domain (*i.e.*, x/D = -40.0). 175 The center of the injection port is located in the middle of the bottom 176 plane, *i.e.*, $(0.0, 0.0, L_z/2.0)$. 177

Taking advantage of the results issued from a preliminary RANS³ com-178 putation of the same geometry [91], the components of the filtered velocity 179 field at the vitiated air inlet are settled from the corresponding computed 180 profiles of the mean velocity components. The value of the boundary layer 181 thickness reported above has been also determined from this computation. 182 The results of the corresponding RANS simulation could have been used to 183 account for velocity fluctuations within the framework of synthetic inlet tur-184 bulence generators. However, some previous analyses devoted to synthetic 185 inlet turbulence have showed that, even with properly set mean velocity and 186 turbulence kinetic energy, the simulated flow fields are quite sensitive to the 187 arbitrary choice of the synthetic turbulence model (e.g., Digital Filter, Ran-188 dom Flow Generator, Synthetic Eddy Model), see for instance [97]. Another 189 strategy may consist in running a concurrent supersonic turbulent boundary 190 layer (STBL) simulation, making use of rescaling and reintroduction pro-191 cedures, with the inflow conditions for the main simulation extracted from 192 a plane of the concurrent STBL simulation. The associated computational 193 costs are however non-negligible. Thus, no special effort has been spent to 194 represent the unsteady (*i.e.*, turbulent) features of the supersonic boundary 195 layer. This choice can be justified (at least partly) on the basis of previous 196 reactive LES conducted on JISCF geometry, which were found able to re-197 produce satisfactorily experimental trends and results without taking inlet 198 velocity fluctuations into account [98, 99]. In any case, it seems worth em-199

²Here, the quantity u denotes the norm of the velocity vector.

³RANS: Reynolds-averaged Navier-Stokes

phasizing that inlet turbulence is completely altered by the wall injection, 200 the resulting bow shock formation and associated flow separation. Moreover, 201 we will see that the present flow conditions lead to a combustion stabilization 202 region located quite far downstream of the upstream injection zone. The tur-203 bulence in this region is thus more likely to be driven by the development of 204 the wake structure (downstream of the JISCF) than by the small scale struc-205 tures of the turbulent boundary layer (upstream of the injection). Therefore, 206 for the purpose of the present study, we follow a strategy similar to the one 207 previously described by Techer *et al.* [81] and a simpler natural development 208 of the turbulent flowfield has been chosen with no fluctuation imposed at the 209 inlet boundary. In regard to the fuel injection, the velocity profile is set with 210 an error function so as to mimic the presence of boundary layers. At the cor-211 responding inlet, the mesh is generated in order to maintain approximately 212 50 points inside the injection diameter with at least five points within the 213 shear layer. No-slip adiabatic wall conditions are used around the fuel injec-214 tion at the bottom of the computational domain. So as to avoid any spurious 215 numerical wave reflections, extrapolation conditions are used in conjunction 216 with grid coarsening at the top, backside, and frontside of the computational 217 domain. Extrapolation rules are applied at the supersonic outlet (*i.e.*, right 218 boundary of the computational domain). Finally, the flow is initialized with 219 the supersonic air inflow conditions in the whole computational domain. The 220 main characteristics of the two inlet streams are gathered in Table 2. The 221 Courant-Friedrichs-Lewy (CFL) number was adjusted between 0.9 and 1.2. 222 Furthermore, in order to investigate the mixing between the hydrogen jet 223 and vitiated air crossflow, we consider a fuel inlet tracer or mixture fraction 224 (*i.e.*, a passive scalar ξ), the value of which is set to zero at the vitiated air 225 inlet and to unity in the hydrogen jet. 226

The simulation is first conducted in non-reactive conditions from t = 0.0227 until $t = t_i = 150.0 D/u_{\infty}$, once the computed flowfield displays a sta-228 bilized compressible flow structure. Then, chemical source terms are acti-229 vated. Combustion chemistry is described using the four-step reduced kinetic 230 scheme of Boivin *et al.* [100], which features six reactive chemical species (H_2, H_2) 231 O_2 , H_2O , H, HO_2 , and H_2O_2) and two additional chemical species (O and 232 OH) that are evaluated from the quasi-steady-state approximation (QSSA). 233 This reduced mechanism has been tested and validated in many elementary 234 test cases [100]. The physical time of the simulation in reactive conditions 235 is about $170.0 D/u_{\infty} = 260.0 \ \mu s$ and, over this period of time, 2250 snap-236 shots are recorded every 0.115 μs , thus capturing the development of ignition 237 processes and combustion stabilization. 238

239

The OH radical molar fractions obtained at three distinct times from

 $t^* = u_{\infty}(t-t_i)/D = 80.0$ to $t^* = 170.0$ are displayed in the mid plane along 240 the spanwise direction (see Fig. 3) and in the plane y/D = 0.25 along the 241 vertical direction (see Fig. 4). From $t^* = 0.0$ to $t^* = 80.0$, the stabilization 242 location is continuously progressing upstream (*i.e.*, towards the hydrogen 243 injection port). Then, from $t^* = 100.0$ to $t^* = 170.0$, as illustrated in 244 Figs. 3 and 4, the leading reactive zone (i.e., the stabilization region) is 245 observed to move back and forth between x/D = 25.0 and x/D = 40.0. The 246 resulting averaged fields — not included due to restriction lengths — exhibit 247 a satisfactory level of convergence. 248

The obtained results also show that the amounts of OH radical present in the 249 recirculation zone upstream of the jet, which is formed just downstream of 250 the bow shock, remain quite small, suggesting that this zone is only weakly 251 reactive. This is in contrast with the levels of OH concentrations obtained 252 in the wake of the jet in the near wall region, which is highly reactive. 253 The corresponding reaction zone spreads over a region that is delineated by 254 z/D = -5.0 and z/D = 5.0, it is however not confined in height and extends 255 beyond the limits of the computational domain. Finally, the most significant 256 levels of heat release rate are obtained in the vicinity of the wall within a 257 sonic region where the equivalence ratio is around two, as it is shown in 258 Fig. 5. 259

²⁶⁰ 3. Preliminary analysis of the non-reactive flowfield

All the results reported in this section have been obtained from the analysis and post-processing of the <u>non-reactive</u> flowfield computation.

In a first step of the analysis, we proceed with the characterization of the 263 unburnt mixture temperature which is essential since it will allow to identify 264 the regions that are prone to the development of ignition processes. In 265 this respect, Gamba and Mungal [101] showed that combustion stabilization 266 in JISCF may take place in various regions of the flow: either upstream 267 or downstream of the injector port, within the mixing layer, and further 268 downstream, in the near-wall region, where chemical reactions were found 269 to be the most significant. Therefore, special attention must be paid to the 270 evaluation of the composition of the mixture (temperature and species mass 271 fractions) in the vicinity of the walls. 272

Figure 6 displays scatterplots of the temperature plotted versus the mixture fraction. In the same picture is also depicted the linear approximation of the temperature evolution, *i.e.*, $T_{\rm u}(\xi) = \xi T_{\rm fuel} + (1.0 - \xi)T_{\rm ox}$, with the couple of values $(T_{\rm fuel}, T_{\rm ox})$ associated to the inlet stream conditions $(T_{\rm jet}, T_{\infty})$, and with ξ the mixture fraction (or fuel inlet tracer). The data significantly

depart from the linear approximation and the variations of thermal capaci-278 ties with temperature are sufficient to explain such departures. Indeed, once 279 plotted versus the mixture fraction, the quantity that could be expected to 280 display such a linear behaviour is the enthalpy or, more precisely, for high-281 speed flows such as the one considered herein, it is the total enthalpy [67, 69]. 282 In this respect, the hydrogen jet ($\xi = 1.0$) undergoes a very high expansion 283 and its temperature first significantly decreases. It is subsequently increased 284 as a consequence of the Mach disk compression. The vitiated air stream 285 $(\xi = 0.0)$ is compressed through the bow shock and its temperature is further 286 increased by viscous dissipation in the direct vicinity of the wall (y/D = 0.0). 287 We will see that it is quite useful to establish a generalized (*i.e.*, non-linear) 288 but approximated expression that relates the fresh reactants temperature to 289 the mixture fraction. For this purpose, a sixth-order polynomial interpola-290 tion is considered: $T_{\rm u}(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + a_4\xi^4 + a_5\xi^5 + a_6\xi^6$ where 291 the quantities a_k $(k = 1, \dots, 6)$ denote the polynomial coefficients (in K). 292 This expression will be used hereafter so as to evaluate some characteristics 293 (e.q., ignition delay and flame propagation velocity) of the unburnt mixture. 294 A preliminary analysis of the ignition processes is first conducted on 295 the basis of the reactivity λ introduced by Boivin *et al.* [103, 104]. The 296 quantity λ is the real positive eigenvalue of the Jacobian that characterizes 297 the differential system describing the changes in concentrations of H, O, and 298 OH. According to its definition, it is inversely proportional to the ignition 299 delay of a homogeneous mixture. More precisely, as shown in Fig. 7, the 300 ignition delay is of the order of $(0.06\lambda)^{-1}$ and can be readily estimated from 301 the values of the temperature, pressure, and concentrations of H_2 and O_2 . 302 Figure 8 displays the parietal field of the reactivity, which allows to put 303 into evidence the regions that are prone to ignition. Downstream of the 304 injection (10.0 < x/D < 150.0), the most reactive regions⁴ are located on 305 both sides of the hydrogen jet wake, as it is confirmed by the isocontour 306 $0.95 \langle \lambda \rangle_{\rm max}$, which is located in the vicinity of the abscissa x/D = 60.0. It 307 is however noteworthy that, upstream of the injection, the reactivity values 308 are even larger, see the top of Fig. 8. In this regard, according to the work 309 of Gamba and Mungal [101] and Vincent-Randonnier et al. [91], it seems 310 that this zone, which is associated to high levels of segregation between 311 fuel and oxidizer, does not allow for ignition and combustion stabilization. 312 This emphasizes the relevance of any modelling proposal, such as the one 313 considered in reference [71], that considers the influence of a Damköhler 314

⁴In this region, the maximum value of the reactivity is $\lambda_{\text{max}} = 434,500 \text{ s}^{-1}$.

number based on the residence time $\tau_{\rm res}$, *i.e.*, $Da = \tau_{\rm res}/\tau_{\rm igni}$, the transport equation of which has been recently derived [105].

317 4. Analysis of the high-speed turbulent combustion regimes

All the results reported in this section have been obtained from the analysis and post-processing of the <u>reactive</u> flowfield computation.

The present geometry corresponds to a separated injection of the fuel in 320 the oxidizer stream but the molecular mixing processes that take place be-321 tween them — before combustion stabilization occurs — lead to a partially 322 premixed mixture. The analysis of the reaction zone will therefore benefit 323 from the evaluation of the degree of premixing between fuel and oxidizer. 324 Thus, with the objective of distinguishing between the two limits of non-325 premixed ($\zeta_p = 0.0$) and premixed combustion ($\zeta_p = 1.0$), a premixedness 326 index ζ_p or flame index (FI) [106, 107] will be considered. It is presently eval-327 uated from $\zeta_p = (1.0 + n_{\rm F} \cdot n_{\rm O})/2.0$, where the quantities $n_{\rm F}$ and $n_{\rm O}$ denote 328 unit vectors normal to iso-contours of the fuel and oxidizer mass fractions, 329 respectively. It will be used to delineate locations that can be identified as 330 premixed regions. As shown in Fig. 9, both premixed and non-premixed con-331 tributions are relevant to the present configuration. An illustration of this 332 distribution is provided in Fig. 10, which depicts the instantaneous flame 333 structure obtained at $t^* = 170.0$. This figure displays both OH and pre-334 mixedness index distributions on the stoichiometric iso-surface. It shows 335 that chemical reactions indeed proceed in a partially premixed combustion 336 mode featuring premixed combustion in the vicinity of the stabilization zone. 337 One may also notice that the water vapor present in the vitiated airstream 338 leads to a slight production of OH radicals at the bow shock location, which 339 is clearly visible on the parietal field of OH concentration displayed at the 340 top of Fig. 10. 341

Since chemical reactions take place rather far downstream of the hy-342 drogen injection port, after molecular mixing proceeds between hydrogen 343 and high temperature vitiated air, combustion develops not only in partially 344 premixed mixtures but also in high temperature conditions, *i.e.*, above the 345 crossover [108]. Therefore, it is essential to attempt to discriminate between 346 two possible physical mechanisms: flame propagation and ignition processes, 347 which may be both involved in combustion stabilization. Thus, a simple pre-348 liminary study has been conducted on the basis of (i) one-dimensional pre-349 mixed flame and (ii) homogeneous reactor computations so as to distinguish 350 between the two phenomena (flame propagation and ignition). These com-351 putations are performed considering various mixtures of fresh reactants at 352

a temperature given by the expression introduced above, *i.e.*, $T_{\text{mix}} = T_u(\xi)$, 353 and since pressure variations were found to remain negligible in the region 354 where chemical reactions proceeds, these computations are performed in iso-355 baric conditions at $p_0 = 56$ kPa, whatever the value of the mixture fraction. 356 Figure 11 displays the evolution of the ignition delay as a function of 357 the mixture fraction ξ (top of the figure) and equivalence ratio Φ (bottom 358 of the figure). The evolution of the unburnt mixture temperature $T_u(\xi)$ 359 is also depicted. It is quite remarkable that the reactivity λ provides an 360 excellent estimate of the ignition delay without requiring any numerical in-361 tegration of the chemical system. Moreover, this set of curves puts into 362 evidence the strong non-linearity of the ignition delay variation with the 363 mixture fraction ξ . This characteristic time is very long for lean mixtures, 364 decreases as the mixture fraction value is increased, until it reaches a local 365 minimum, *i.e.*, the most reactive condition [109], and then sharply increases 366 for richer mixtures. The most reactive state (*i.e.*, $\xi_{\rm mr}$), which is estimated 367 from the minimum ignition delay time, does not correspond to stoichiometry 368 (*i.e.*, ξ_{st} or $\Phi = 1.0$) but to a mixture fraction value that is approximately 369 equal to 0.0065 (*i.e.*, $\Phi_{\rm mr} = 0.207$). This is a direct consequence of the sig-370 nificant temperature difference between the (cold) fuel stream and the (hot) 371 oxidizer stream. It is also remarkable that the self-ignition delay displays 372 a sharp increase for rich conditions in such a manner that spontaneous ig-373 nition regimes are less likely for these rich mixtures. More precisely, the 374 corresponding ignition regimes require more time to develop, which may fa-375 vor flame propagation mechanism. We will see below that flame propagation 376 time scales indeed remain significantly smaller than ignition delays for such 377 rich mixtures. However, as long as lean conditions are considered, only the 378 ignition processes are expected to occur. 379

Figure 12 reports the evolution of the planar unstrained premixed lami-380 nar flame speed S_L^0 and its thermal thickness δ_L^0 as a function of the mixture 381 fraction. This figure complements Fig. 11 in terms of the mixture frac-382 tion variation domain $\xi \in [0.0, 1.0]$. Indeed, in Fig. 12, only the domain 383 $\xi \in [0.04, 0.30]$ is represented since, below the minimum bound, only igni-384 tion processes become relevant. Indeed, beyond this limit, the values of the 385 laminar flame speed and thickness display unphysical variations from one 386 computation to another and the corresponding results strongly depend on 387 numerical simulation parameters (computational domain length, number of 388 points, time-step, etc.) Finally, on the other side, beyond the maximum 389 limit, the laminar flame speed tends towards zero: the high flammability 390 limit is reached. The flame propagation velocity is indeed significantly de-391 creased as the mixture fraction is increased beyond 0.3. It should reach 392

a maximum (together with a minimum flame thickness) in the vicinity of
stoichiometry or most reactive condition but the ignition mechanism is the
leading and controlling process for these mixtures.

396 4.1. Turbulent combustion regimes in the Barrère-Borghi coordinates

In order to determine the variability of the premixed combustion regime 397 in the present JISCF configuration, the data are first displayed as a scatter-398 plot in a diagram that is commonly referred to as the Borghi diagram. The 399 corresponding set of coordinates, introduced in reference [73, 111–113], cor-400 responds to (i) a dimensionless velocity ratio u'/S_L^0 , with u' (or $u_{\rm rms}$) the 401 root-mean-square (RMS) of velocity fluctuation normalized by the laminar 402 flame propagation velocity S_L^0 , and *(ii)* a dimensionless length scale ratio 403 L_t/δ_L^0 , *i.e.*, the turbulent integral scale L_t normalized by the laminar flame 404 thickness δ_L^0 . In the following, the characteristic velocity fluctuation u' os 405 evaluated from the resolved turbulent kinetic energy k, *i.e.*, $u' = \sqrt{2k/3}$, 406 and the integral length scale L_t is estimated from $L_t = u'^3/\varepsilon$ with ε the 407 resolved dissipation rate. 408

To proceed with the construction of this diagram the characteristics of 409 the laminar premixed flame, *i.e.*, S_L^0 and δ_L^0 , are evaluated only in a re-410 stricted part of the computational domain which is associated to (i) a prob-411 ability that the flame index ζ_p exceeds a threshold value⁵ larger than ten 412 percent (this quantity is hereafter denoted by P_{PCZ}) and (ii) mixture frac-413 tion values ξ within the range [0.04, 0.3] which, according to Fig. 12, corre-414 spond to reactive mixtures within which a premixed flame may propagate. 415 This is in contrast with most of previous analyses of turbulent combustion 416 regimes [114–117] where the corresponding quantities, *i.e.*, S_L^0 and δ_L^0 , were 417 generally evaluated from one single condition in terms of equivalence ratio, 418 operating pressure, and fresh reactants temperature. 419

The corresponding set of data is presented in Fig. 13. This figure shows 420 that, at z/D = 0.0 (see Fig. 13(c)), premixed combustion regimes are highly 421 variable from one location to another. Possible combustion regimes include 422 quasi-laminar premixed flame, thick flames, thickened flames, and thickened-423 wrinkled flames. In the near-wall region (y/D = 0.0 and y/D = 0.25), the 424 laminar flame regimes predominate, see Figs. 13(a) and 13(b). Overall, the 425 most significant heat release rate (HRR) values are associated to a Damköh-426 ler number smaller than unity. The turbulence time scales are rather small 427 compared to the chemical time scales that are deduced from the flame propa-428

⁵The threshold value ζ_p^{lim} is set to 0.7.

gation characteristics: chemistry can be considered as slow. The most probable regimes are associated to values of the Karlovitz number $\text{Ka} = (\delta_L^0/\eta)^2$ that are significantly larger than unity: the thin flame assumption does not hold. Farther from the wall and injection port, the present set of results shows that values of the Damköhler number Da can exceed unity and that wrinkled flame regimes can be reached.

The scatterplot issued from the data collected in the medium plane 435 (z/D = 0.0), see Fig. 13(c), is quite similar to the one issued from the 436 Reynolds-averaged Navier-Stokes numerical simulation of the HIFiRE Di-437 rect Connect Rig geometry conducted by Quinlan et al. [77]. Compared to 438 our results, the sole remarkable difference is a slight shift of the distribution 439 upwards on the right; the distribution reported by Quinlan et al. [77] fea-440 tures a *tongue* in the neighborhood of $(L_t/\delta_L^0, u'/S_L^0) = (0.10, 10.0)$ following the isoline Ka = 100.0 up to values of L_t/δ_L^0 approximately equal to one hun-441 442 dred. As shown in the scatterplot gathered at z/D = 0.0 (see Fig. 13), the 443 distribution issued from our own computational data features a quite similar 444 tongue but it is following the isoline Ka = 20.0 (instead of Ka = 100.0). 445 This dissemblance may be readily explained by the differences in terms of 446 geometry (including cavities, multiple injections, etc.) and operating point 447 (pressure, temperature, equivalence ratio, and fuel). 448

Together with those previously obtained by Quinlan *et al.* [77], the present results show that the wall boundary conditions significantly influence the dispersion of the observed premixed turbulent combustion regimes. In particular, it seems that the Karlovitz number value remains almost constant in the direct vicinity of the wall and the corresponding value is expected to depend on the studied configuration.

455 4.2. Turbulent combustion regimes in the (Re_t, Da) -coordinates

To complete the above combustion regime analysis, which was focused on 456 the premixed flame propagation mode, we consider now turbulent combus-457 tion diagrams based on the couple (Re_t, Da) . The corresponding represen-458 tation is often referred to as the Williams coordinates. The most probable 459 domains associated with supersonic combustion regimes, delineating the op-460 erating range of scramjets, were previously analyzed in such diagrams by 461 Balakrishnan and Williams [75] and Ingenito and Bruno [76]. The corre-462 sponding domains will be depicted with red, blue, and green dotted lines in 463 the figures discussed below. The definition of these domains are based on the 464 consideration of a flight Mach number value that lies between 1.0 and 4.0 in 465 reference [75] while the values 7.0–9.0 were considered in reference [76]. Tem-466 perature values within the range 300.0 - 1200.0 K were retained in the anal-467

ysis conducted by Balakrishnan and Williams [75], while a value of 1000.0 K 468 was used in reference [76]. Balakrishnan and Williams considered very high 469 levels of turbulence intensity in the combustion chamber (*i.e.*, up to 50.0 %) 470 while values 0.5 - 10.0 % were retained as relevant ones in reference [76]. For 471 the integral scale L_t , Balakrishnan and Williams [75] considered the dimen-472 sions of the combustion chamber as a reference length scale and chemical 473 scales were determined from strained diffusion flamelets. The most probable 474 supersonic combustion regimes, *i.e.*, those that are likely to be encountered in 475 scramjets, were thus delineated [75]. However, as stated by the authors, this 476 does not take into account the possible influence of the heat release on the 477 turbulent kinetic energy, an influence that would lead to its decrease through 478 the temperature-induced increase in viscosity. Lastly, there were still some 479 uncertainties about the possible effects of ignition, which could alter the low 480 limit of the possible supersonic combustion range. Ingenito and Bruno [76] 481 defined this possible domain of supersonic combustion regimes through the 482 analysis of single-step chemistry LES computations of the SCHOLAR bench-483 mark. To conclude this brief introduction, it should be acknowledged that 484 there are some uncertainties that remain regarding the possible impact of 485 the fuel injection strategy and combustion chamber geometry, which has 486 a significant influence on the mixing processes development and resulting 487 Damköhler number values. As shown by Berglund *et al.* [118, 119], it is 488 possible to evolve from flamelet regimes to distributed combustion regimes 489 by switching from one configuration to another. The conclusions of such 490 combustion regime studies are also expected to depend on the specification 491 of boundary conditions. 492

From a general viewpoint, the Damköhler number, which is used as the 493 ordinate in the combustion diagram, is estimated from $Da = \tau_t / \tau_c$ with 494 $\tau_t = L_t/u'$, the large eddy turnover time and τ_c , a chemical time scale. In 495 the following, we will consider three distinct possibilities for estimating the 496 value of this chemical time scale, which will be based (i) on the water vapor 497 production rate, (ii) on the laminar premixed flame transit time δ_L^0/S_L^0 , and 498 (iii) on the ignition delay as deduced from the reactivity λ [103, 104]. These 499 various time scales make possible the definition of Damköhler number based 500 on (i) water vapor production rate (Da_{H_2O}) , (ii) flame propagation mecha-501 nisms (Da_L) , and *(iii)* ignition processes (Da_i) , respectively. The turbulent 502 Reynolds number, which appears as the abscissa of the combustion diagram, 503 will be evaluated from $\operatorname{Re}_t = L_t u' / \langle \nu \rangle = k^2 / \langle \nu \rangle \varepsilon$. 504

In a first step of this analysis, we consider a diagram based on the same definition as the one previously retained by Ingenito and Bruno [76]: we use the inverse of the production rate of water vapor as the relevant chemical

time scale. Figure 14 presents the corresponding (Re_t, Da_{H_2O}) combustion 508 diagram. It shows that the obtained supersonic combustion regimes lie below 509 the zone delineated by Ingenito and Bruno [76]. This result is fully consistent 510 with the study of Cock [120] who scrutinized the effects (on Damköhler 511 number estimates) of a multi-step finite-rate chemical kinetics description 512 compared to a single-step chemistry. The large gap, of about two decades, 513 that is observed between the present set of results and those documented in 514 reference [76], is thus ascribed to the use of a finite-rate multi-step chemistry. 515 Moreover, the present set of results lies in the vicinity of the low boundary 516 (*i.e.*, minimum bounds in Re_t and Da_{H_2O}) of the possible domain defined by 517 Balakrishnan and Williams [75], which is depicted in blue color in Fig. 14. 518 At this level, it is noteworthy that, as emphasized by Balakrishnan and 519 Williams, the main effect of heat release is to reduce the turbulent kinetic 520 energy, an effect that has not been considered in the delineation of the cor-521 responding domain in reference [75]. The work of Cock [120] and the more 522 recent analysis of Fureby [121] also documented the way the heat release 523 may alter the turbulence intensity in high-speed flow conditions. The results 524 of reference [121] feature very large compressibility effects, with turbulent 525 Mach number values of the order of 1.5 while the turbulent Reynolds num-526 ber values lie between 10^2 and 10^4 . In the present conditions, a decrease in 527 the turbulence intensity from ten to five percent is observed across the reac-528 tive zone. This is in good agreement with the observations made by Ingenito 529 and Bruno [76] but it should be however emphasized that larger turbulence 530 intensity can be expected in confined conditions. 531

In a second step of the analysis, a Damköhler number based on the flame 532 propagation mechanism is considered. The resulting (Re_t, Da_L) diagram 533 is reported in Fig. 15. The regions that are not representative of a flame 534 propagation mechanism are excluded from the analysis by using the same 535 conditioning (based on the premixedness probability and mixture fraction 536 limits) as the one introduced in the previous subsection. Figure 15 shows 537 that, in comparison to the data presented above, the scatterplot has been 538 translated upwards by about one decade to reach the broken flamelets regime, 539 above the slow chemistry limit $Da_L = 1.0$ limit. The tapered shape of the 540 scatterplot follows the isoline $Ka_L = 100.0$. It is noteworthy that this dif-541 fers from the regimes delineated above in the Barrère-Borghi coordinates. 542 This is just a consequence of the unity flame Reynolds number assump-543 tion, *i.e.*, $S_L^0 \delta_L^0 / \nu = 1.0$, which is not perfectly verified; the boundaries that 544 are delineated in the Borghi diagram are indeed based on this assumption, 545 which is used to relate the Damköhler, Karlovitz, and Reynolds numbers: 546 $\operatorname{Re}_t = \operatorname{Da}_L^2 \operatorname{Ka}_L^2$. The scatterplot reaches the regions that were previously 547

delineated for supersonic combustion regimes in the studies of Balakrishnan
and Williams [75] and Ingenito and Bruno [76]. Most of the heat release
rate takes place in the PSR regime as already shown above in the premixed
turbulent combustion diagram (see Fig. 13).

The diagram displayed in Fig. 15(a) shows that the points where the 552 probability to lie within a premixed combustion zone is the most important 553 are gathered around the isoline $Da_L = 1.0$ and lie within the broken flamelets 554 regime, which can be associated to thickened-wrinkled flame regime in the 555 Barrère-Borghi coordinates. This region is also characterized by supersonic 556 flow conditions (*i.e.*, Ma > 1.0). In this respect, the combustion diagram 557 reported in Fig. 15(c) also indicates that the sonic line follows closely the 558 low limit of the supersonic combustion regimes delineated by Ingenito and 559 Bruno [76]. As pointed out by Balakrishnan and Williams [75], this dia-560 gram does incorporate neither the compressibility nor the high-Mach num-561 ber effects, which can be important in high-speed flow conditions. Thus, 562 the turbulent Mach number, which provides a measure of compressibility 563 effects on turbulence, has been also considered. Its value is significant (be-564 tween 0.2-0.3) in regions where the heat release rate is highest, *i.e.*, in the 565 vicinity of the wall (y/D < 1.0), then it decreases in the regions that are 566 associated to the broken flamelet regime. At this level, it is noteworthy that 567 Fureby [121] has conducted a similar analysis on the HyShot II configura-568 tion. In this study important compressibility effects were put into evidence, 569 with turbulent Mach number values that can be locally as high as 1.5. The 570 corresponding regions are under the influence by the counter-rotating vor-571 tices pair (CVP), shock reflection, and shock-induced ignition. Indeed, in 572 the simulated geometry, the shock train certainly allows for the persistence 573 of a high level of velocity fluctuations at each reflected shock wave crossing. 574 Finally, the last two diagrams reported in Figs. 15(e) and 15(f) display the 575 scatterplots colored by the normalized coordinates and thus allow to identify 576 the flow regions in which the various turbulent combustion regimes develop. 577 In the near wall region and in the vicinity of the injection port, the com-578 bustion regime is mostly that of a PSR, while farther from the wall and 579 hydrogen injection, the broken flamelets regime is the most probable. 580

The combustion regime analysis is ended by considering a Damköhler number definition that is based on the ignition delay. The resulting turbulent combustion diagrams are displayed in Fig. 16. Since the corresponding definition does not account for any flame structure (the retained time scale is indeed deduced from homogeneous reactor computations), the regimes relevant to such flame structures are no longer referred to in these diagrams. Thus, only three sub-domains are considered: the laminar regime, the PSR

or slow chemistry regime, and the fast chemistry regime. Compared to the 588 previous set of diagrams, the scatterplots displayed in Fig. 16 exhibit some 589 thickening since the number of points under consideration has been signifi-590 cantly increased: the sole conditioning that is applied corresponds to a sim-591 ple thresholding of the heat release rate (one tenth percent of its maximum 592 value). First, it is noteworthy that the scatterplot has been translated up-593 wards by about one decade in comparison with the previous results obtained 594 with a Damköhler number definition based on laminar premixed flamelets. 595 The distribution features larger values of the Damköhler number. This con-596 firms that, even if combustion takes place in the direct vicinity of the wall, 597 the principal mechanism for combustion stabilization is related to ignition 598 rather than flame propagation. One can also notice that the elongated part 599 of the distribution now varies between $Ka_i = 1.0$ and $Ka_i = 20.0$. Moreover, 600 it is quite remarkable that, with the present definition of the Damköhler 601 number, the scatterplots is in satisfactory agreement with supersonic com-602 bustion regime regions previously delineated by Ingenito and Bruno [76] and 603 by Balakrishnan and Williams [75]. In contrast to the previous set of data 604 relevant to premixed flame propagation (see Fig. 15), the present set of re-605 sults — which does account for the contribution of ignition processes – 606 shows that the most important HRR values are associated to fast chemistry 607 regimes featuring $1.0 < Da_i < 100.0$. Figure 16(a) also confirms that the 608 regions associated to significant HRR values correspond to moderate SDR 609 (with the SDR evaluated from its resolved contribution), *i.e.*, conditions 610 which are favourable to the development of ignition processes [109]. 611

The inspection of the Mach number shows that the fast chemistry regimes ($1.0 < Da_i < 100.0$) are relevant to supersonic flow conditions (Ma > 1.2). The turbulent Mach number values indicate that the compressibility effects are important in the near wall region y/D < 1.0, *i.e.*, in regions featuring significant heat release rates.

⁶¹⁷ 5. Conclusions and prospects

High-speed turbulent combustion regimes are analyzed in standard com-618 bustion diagrams based on (i) either the Barrère-Borghi coordinates or (ii) 619 in the (Re_t, Da) -plane, which is often referred to as the Williams coordinates. 620 Since they rely on dimensional reasoning and scaling principles, the various 621 boundaries that delineate the corresponding regimes have been early and 622 continuously questioned over the years [122, 123]. In this respect, it seems 623 worth recalling that such diagrams were introduced almost fifty years ago so 624 as to provide a rather qualitative view of the possible evolution of turbulent 625

combustion interactions as the characteristic length and time scales of the 626 turbulent flowfield and/or chemistry are varied. Despite the intrinsic limi-627 tations of this overly simplified picture of turbulence-chemistry interactions, 628 such heuristic diagrams do provide a quite valuable point of view and it is 629 quite remarkable that, still today, they are retained as a first useful step 630 to characterize turbulent combustion setups and they concentrate a signifi-631 cant amount of research works. For instance, some insights onto the limit of 632 flamelet broadening have been recently gained from experimental and compu-633 tational studies of premixed flames subject to intense turbulence [124, 125]. 634 The interaction of high-speed turbulence with premixed flames has been 635 also investigated by Poludnenko and Oran [126, 127] and several DNS stud-636 ies have been focused on combustion regimes featuring large values of the 637 Karlovitz number [128–131]. For such conditions, it is quite remarkable that, 638 in contrast to the standard picture of thickened flame regimes, some local 639 thicknesses (e.g., norms of the species mass fraction gradient of intermediate 640 species like carbon monoxide) do exhibit thinning rather than broadening 641 effects. Moreover, in contrast to the picture of a large and nearly homoge-642 nous reaction zone, high-fidelity imaging of the flame structure and topology 643 has shown that extreme turbulence may lead to the formation of distributed 644 reaction pockets (or blobs) that are connected by thin flamelets [132, 133]. 645 As emphasized in reference [134], such a topology displays some similarities 646 with the Shchetinkov's picture of micro-volume combustion regime and his 647 early analysis of combustion processes in a scramiet [135, 136]. 648

In comparison to these studies, which are mostly concerned with fully-649 premixed combustion in low Mach number flows, the present analysis is 650 conducted in conditions relevant to scramjet operations with a separated 651 injection of the fuel in a supersonic vitiated airstream. The consideration 652 of such conditions rises some specific issues. For instance, additional effects 653 related to high Mach number values and compressibility may be expected, 654 which require in principle the extension of combustion diagrams to additional 655 dimensions. However, the Damköhler and Reynolds numbers, *i.e.*, the ratio 656 of flow to chemical time (or lenght) scales are deemed the two most signifi-657 cant parameters. Thus, the difficulty of multi-dimensional diagrams (with a 658 number of dimensions larger than two) is presently circumvented by consid-659 ering combustion regime scatterplots in the standard sets of coordinates but 660 colored by other relevant quantities: Ma, Ma_t , SDR, etc. In addition to this, 661 various Damköhler number definitions have been considered based on either 662 premixed flame propagation or ignition characteristics so as to evaluate rel-663 evant time and length scales. Whatever the definition, this analysis puts 664 into evidence turbulent combustion regimes featuring significant finite-rate 665

chemical kinetics effects. The obtained results show the wide variety of com-666 bustion regimes involved in such high-speed flow conditions. Most of them 667 have however something in common : they lie above the Klimov-Williams 668 limit (Ka > 1.0). This analysis also reveals that, for the conditions that are 669 studied, the largest values of the HRR are obtained in the vicinity of the 670 wall (y/D < 1.0). At the corresponding locations, the reactive mixture fea-671 tures a significant level of premixing. These conditions are also associated 672 to the largest values of the turbulent Mach number (Ma_t ranges between 673 (0.12) and (0.35) and correspond to almost sonic conditions. This emphasizes 674 the relevance of future work devoted to the wall physics (heat transfer, wall 675 roughness, etc.). The influence of wall boundary conditions indeed remains 676 to be more largely addressed since it can significantly affect the near wall 677 flow dynamics of recirculation regions interacting with redeveloping bound-678 ary layers. From a more general point of view, the effects of the confinement 679 (e.q., shock reflection and interaction, resulting SWBLI, etc.) also deserve 680 to be analyzed. 681

To conclude, the physics of high-speed turbulent combustion regimes is 682 not the sole concern in the application of supersonic combustion for possi-683 ble future hypersonic flight. Combustion in scramjet rise other challenging 684 issues for better optimizing the ratio of residence time over chemical times 685 while ensuring stabilization of combustion. Fundamental physical aspects 686 related to compressibility effects competing with significant heat release, af-687 fecting in a different way both large and small turbulent scales need to be 688 addressed. In particular the control of combustion stabilization mechanisms 689 in high-speed reacting flows first requires a deeper understanding of the nu-690 merous sources of unsteadiness associated to shock wave/mixing layers or 691 shock wave/boundary layers interactions (SWBLI). A competition between 692 so-called compressibility effects, reducing the spreading rate of free shear 693 layers, heat release and/or, on the contrary, enhancement of large-scale in-694 stability modes in injection jet for particular physical or geometrical condi-695 tions can tremendously affect the subsequent mixing of reactants. Combined 696 with experiments, the use of high-fidelity tools should be intensified to get 697 further insights into these complex interactions and possibly improve the 698 efficiency of low-order models for optimization. Answering the above issues 699 may require some modelling efforts. For instance, most of the sub-grid scale 700 turbulence and multi-regime combustion models have never been assessed for 701 such extreme conditions. Finally, the relevance of existing chemical kinetics 702 descriptions should also be questioned for these rapidly-variable temperature 703 and pressure conditions. 704

705

The above lines have been written to pay tribute to K.N.C. Bray's con-706 tribution in the field of turbulent combustion modelling. The focus has 707 been placed on combustion in supersonic flows, a topic on which his input 708 in the seventies and nineties was also significant. Before concluding this 709 manuscript, it seems worth emphasizing that Professor Bray is not only rec-710 ognized to be one amongst the most prominent and renowned scientists in 711 the international combustion community, he is also one amongst its most 712 appreciated figures: an eminent scientist who is known as a gentleman. 713

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Fig. 1. Top: three-dimensional schematic view of the flow topology of the underexpanded jet in supersonic crossflow (JISCF). Bottom: definition of the computational domain and associated boundary conditions.



Fig. 2. Computational mesh overview (one single line depicted for six successive nodes).



Fig. 3. Temporal evolution in the median plane z/D = 0.0 of the molar fraction of hydroxyl radical displayed together with a numerical Schlieren, from top to bottom, $t^* = 80.0, 100.0, \text{ and } 170.0.$



Fig. 4. Temporal evolution in the median plane y/D = 0.25 of the molar fraction of hydroxyl radical displayed together with a numerical Schlieren, from top to bottom, $t^* = 80.0, 100.0, \text{ and } 170.0.$



Fig. 5. Distribution of the combustion regime (subsonic / supersonic) evaluated in conditions featuring a HRR value that exceeds one percent of its maximal value $\dot{\omega}_{T,\text{max}}$. The equivalence ratio is plotted versus the Mach number and the distribution is colored by the averaged HRR.



Fig. 6. Scatterplots of the unburnt mixture temperature obtained at $t = t_i = 150.0D/u_{\infty}$ plotted versus the mixture fraction as extracted from planes x/D = 0.0, 25.0, 50.0, and 100.0 together with the corresponding conditional average (continuous black line) and with the linear approximation (black dashed line). The dots are colored by normalized coordinates y/D (top) and z/D (bottom).



Fig. 7. Scatterplots of the reactivity λ plotted versus the mixture fraction in the direct vicinity of the injection (-10.0 < x/D < 10.0; red dots) and downstream of the injection (10.0 < x/D < 110.0; green dots). Comparison between PSR computations of *(i)* the ignition delay using the chemical scheme of Ó Connaire *et al.* [102] (dashed line) and *(ii)* reactivity λ using the reduced chemistry of Boivin *et al.* [100].



Fig. 8. Parietal field of the averaged reactivity $\langle \lambda \rangle$ (s⁻¹). Zoom on the injection (top) and general view (bottom). The isoline $0.95 \langle \lambda \rangle_{max}$ is depicted with a white line.



Fig. 9. Analysis of the non-premixed and premixed modes contributions evaluated in computational cells featuring a HRR value that exceeds one percent of its maximal value $\dot{\omega}_{T,\max}$ at times $t^* = 20.0, 40.0, 60.0, 80.0, 100.0, \text{ and } 170.0$. Top: probability density function (PDF) of the premixedness index. Bottom: conditional average of the normalized HRR plotted versus the premixedness index.



Fig. 10. Instantaneous flame structure at $t^* = 170.0$. Top: iso-surface of the stoichiometric mixture fraction colored by the OH molar fraction and parietal field of the same quantity. Bottom: iso-surface of the stoichiometric mixture fraction colored by the premixedness index. The grey iso-surface corresponds to the mixture fraction $\xi = 0.5$.



Fig. 11. Ignition delay time t_{igni} plotted versus the mixture fraction ξ (top) and equivalence ratio Φ (bottom) with a range of variation equivalent to $\xi \in [3.0 \cdot 10^{-4}, \xi_{\text{st}}]$. Comparison between the results obtained with the detailed mechanism of \acute{O} Connaire *et al.* [102], the reduced mechanism of Boivin *et al.* [100], and the reactivity λ , which is obtained at the initial time of computation. The estimate of the combustion stabilization abscissa is deduced from $x_{\text{igni}} = 0.6u_{\infty}t_{\text{igni}}$.



Fig. 12. Laminar flame velocity S_L^0 and thickness δ_L^0 (top) and flame transit time δ_L^0/S_L^0 (bottom) as a function of the mixture fraction ξ (and global equivalence ratio Φ). Computations performed with the detailed mechanism of Jachimowski *et al.* [110].



Fig. 13. Combustion regime scatterplots in the Barrère-Borghi coordinates. Data are collected in plane y/D = 0.0 (Fig. 13(a)), in plane y/D = 0.25 (Fig. 13(b)), in the longitudinal median plane z/D = 0.0 (Fig. 13(c)), and in cross-stream planes x/D = 25.0, 50.0, 75.0, 100.0, and 125.0 (Fig. 13(d)). Dots are colored by the heat release rate.



Fig. 13. Cont'd.



Fig. 14. Turbulent combustion diagram (Re_t , $\text{Da}_{\text{H}_2\text{O}}$) with a chemical time scale deduced from the water vapor production rate. Data are collected in the median plane (z/D = 0.0). Dots are colored by the heat release rate. The red frame corresponds to the supersonic combustion regimed defined by Ingenito and Bruno [76]. The blue and green frames stand for the possible and most probable domains introduced by Balakrishnan and Williams [75].



Fig. 15. Turbulent combustion diagrams ($\operatorname{Re}_t, \operatorname{Da}_L$) with a chemical time scale deduced from the laminar premixed flame transit time δ_L^0/S_L^0 . Data are collected in the median plane (z/D = 0.0). Dots are colored by (i) the heat release rate (Fig. 15(a)), (ii) probability that the premixedness index exceeds 0.7 (Fig. 15(b)), (iii) Mach number Ma (Fig. 15(c)), (iv) turbulent Mach number Ma_t (Fig. 15(d))), (v) normalized streamwise coordinate x/D (Fig. 15(e)), and (vi) normalized wall-normal coordinate y/D (Fig. 15(f)).



Fig. 15. Cont'd.



Fig. 15. Cont'd.



Fig. 16. Turbulent combustion diagrams ($\operatorname{Re}_t, \operatorname{Da}_i$) with a chemical time scale deduced from the reactivity λ . Data are collected in the median plane (z/D = 0.0). Dots are colored by (i) the heat release rate (Fig. 16(a)), (ii) the SDR (Fig. 16(b)), (iii) Mach number Ma (Fig. 16(c)), (iv) turbulent Mach number Ma_t (Fig. 16(d))), (v) normalized streamwise coordinate x/D (Fig. 16(e)), and (vi) normalized wall-normal coordinate y/D(Fig. 16(f)).



Fig. 16. Cont'd.



Fig. 16. Cont'd.