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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 H_2O , (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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1 **1. General introduction**

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

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

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

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

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

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

53 In comparison with their low-speed counterparts, reactive high-speed
54 flows indeed raise some specific issues. For instance, these reactive high-
55 speed flows do involve some special couplings between chemical reactions and
56 compressibility effects, *i.e.*, compression waves and rarefaction waves. This
57 is because the gas temperature is sensitive to these compression/rarefaction
58 waves. Thus, there is a permanent exchange between internal energy (molec-
59 ular scale) and kinetic energy (macroscopic scale). In this respect, it does
60 not seem useless to remind here that the Mach number Ma is the squared
61 root of the ratio between the kinetic energy (of the flow) and thermal energy
62 or static enthalpy, *i.e.*, the average kinetic energy of molecules. In the vicin-
63 ity of sonic conditions ($Ma = 1$), the kinetic energy is indeed already of the
64 same order of magnitude as the static enthalpy per unit mass and it becomes
65 the main contribution as the Mach number value is increased beyond unity.
66 Therefore, since the kinetic energy dissipation induced by molecular viscos-
67 ity effects, in boundary layers, shear layers or shock waves, is proportional
68 to the squared Mach number Ma^2 , moderate changes in velocity result in
69 non-negligible changes in static temperature and pressure. Considering the
70 sensitivity of chemical reactions to temperature and pressure, this induces a
71 coupling between the velocity field and chemical reactions. The considera-
72 tion of these effects therefore appears as one amongst the specific challenges
73 of high-speed turbulent combustion modelling and the early works of Bray
74 and his coworkers [66, 67] has served as a basis to some of the seldom mod-
75 elling proposals that attempted to address this issue [68–72]. In this respect,

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

81 The manuscript is organized as follows: the next section (Sec. 2) provides
 82 a brief overview of the computational database that is used to proceed with
 83 the present investigation ; it is followed by a short section (Sec. 3) where some
 84 features of the unburnt mixture (temperature and reactivity) are scrutinized.
 85 The analysis of high-speed combustion regimes, which is the core of the
 86 present study, is detailed in Sec. 4. Finally, perspectives for future works are
 87 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

88 2. Overview of the computational setup and database

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

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

	hydrogen jet	vitiated airstream
ξ (-)	1.0	0.0
Y_{H_2} (-)	1.0	0.0
Y_{O_2} (-)	0.0	0.2527
$Y_{\text{H}_2\text{O}}$ (-)	0.0	0.1631
Y_{N_2} (-)	0.0	0.5842
p / p_0 (Pa / Pa)	502,918 / 958,055	56000 / 409000
T / T_0 (K / K)	248 / 300	1108 / 1695
ρ ($\text{kg}\cdot\text{m}^{-3}$)	0.490	0.161
γ (-)	1.42	1.27
Ma (-)	1.0	2.0
u ($\text{m}\cdot\text{s}^{-1}$)	1204	1313
m ($\text{g}\cdot\text{s}^{-1}$)	1.85	146.55

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

¹Further detail about the BC specification is provided below.

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

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

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

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

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

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

The simulation is first conducted in non-reactive conditions from $t = 0.0$ until $t = t_i = 150.0 D/u_\infty$, once the computed flowfield displays a stabilized compressible flow structure. Then, chemical source terms are activated. Combustion chemistry is described using the four-step reduced kinetic scheme of Boivin *et al.* [100], which features six reactive chemical species (H_2 , O_2 , H_2O , H , HO_2 , and H_2O_2) and two additional chemical species (O and OH) that are evaluated from the quasi-steady-state approximation (QSSA). This reduced mechanism has been tested and validated in many elementary test cases [100]. The physical time of the simulation in reactive conditions is about $170.0 D/u_\infty = 260.0 \mu s$ and, over this period of time, 2250 snapshots are recorded every $0.115 \mu s$, thus capturing the development of ignition processes and combustion stabilization.

The OH radical molar fractions obtained at three distinct times from

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

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

260 3. Preliminary analysis of the non-reactive flowfield

261 All the results reported in this section have been obtained from the anal-
 262 ysis and post-processing of the non-reactive flowfield computation.

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

273 Figure 6 displays scatterplots of the temperature plotted versus the mix-
 274 ture fraction. In the same picture is also depicted the linear approximation
 275 of the temperature evolution, *i.e.*, $T_u(\xi) = \xi T_{\text{fuel}} + (1.0 - \xi) T_{\text{ox}}$, with the cou-
 276 ple of values $(T_{\text{fuel}}, T_{\text{ox}})$ associated to the inlet stream conditions $(T_{\text{jet}}, T_\infty)$,
 277 and with ξ the mixture fraction (or fuel inlet tracer). The data significantly

278 depart from the linear approximation and the variations of thermal capaci-
 279 ties with temperature are sufficient to explain such departures. Indeed, once
 280 plotted versus the mixture fraction, the quantity that could be expected to
 281 display such a linear behaviour is the enthalpy or, more precisely, for high-
 282 speed flows such as the one considered herein, it is the total enthalpy [67, 69].
 283 In this respect, the hydrogen jet ($\xi = 1.0$) undergoes a very high expansion
 284 and its temperature first significantly decreases. It is subsequently increased
 285 as a consequence of the Mach disk compression. The vitiated air stream
 286 ($\xi = 0.0$) is compressed through the bow shock and its temperature is further
 287 increased by viscous dissipation in the direct vicinity of the wall ($y/D = 0.0$).
 288 We will see that it is quite useful to establish a generalized (*i.e.*, non-linear)
 289 but approximated expression that relates the fresh reactants temperature to
 290 the mixture fraction. For this purpose, a sixth-order polynomial interpola-
 291 tion is considered: $T_u(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + a_4\xi^4 + a_5\xi^5 + a_6\xi^6$ where
 292 the quantities a_k ($k = 1, \dots, 6$) denote the polynomial coefficients (in K).
 293 This expression will be used hereafter so as to evaluate some characteristics
 294 (*e.g.*, ignition delay and flame propagation velocity) of the unburnt mixture.

295 A preliminary analysis of the ignition processes is first conducted on
 296 the basis of the reactivity λ introduced by Boivin *et al.* [103, 104]. The
 297 quantity λ is the real positive eigenvalue of the Jacobian that characterizes
 298 the differential system describing the changes in concentrations of H, O, and
 299 OH. According to its definition, it is inversely proportional to the ignition
 300 delay of a homogeneous mixture. More precisely, as shown in Fig. 7, the
 301 ignition delay is of the order of $(0.06\lambda)^{-1}$ and can be readily estimated from
 302 the values of the temperature, pressure, and concentrations of H₂ and O₂.
 303 Figure 8 displays the parietal field of the reactivity, which allows to put
 304 into evidence the regions that are prone to ignition. Downstream of the
 305 injection ($10.0 < x/D < 150.0$), the most reactive regions⁴ are located on
 306 both sides of the hydrogen jet wake, as it is confirmed by the isocontour
 307 $0.95 \langle \lambda \rangle_{\max}$, which is located in the vicinity of the abscissa $x/D = 60.0$. It
 308 is however noteworthy that, upstream of the injection, the reactivity values
 309 are even larger, see the top of Fig. 8. In this regard, according to the work
 310 of Gamba and Mungal [101] and Vincent-Randonnier *et al.* [91], it seems
 311 that this zone, which is associated to high levels of segregation between
 312 fuel and oxidizer, does not allow for ignition and combustion stabilization.
 313 This emphasizes the relevance of any modelling proposal, such as the one
 314 considered in reference [71], that considers the influence of a Damköhler

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

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

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

318 All the results reported in this section have been obtained from the anal-
319 ysis and post-processing of the reactive flowfield computation.

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

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

353 a temperature given by the expression introduced above, *i.e.*, $T_{\text{mix}} = T_u(\xi)$,
 354 and since pressure variations were found to remain negligible in the region
 355 where chemical reactions proceeds, these computations are performed in iso-
 356 baric conditions at $p_0 = 56$ kPa, whatever the value of the mixture fraction.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

508 time scale. Figure 14 presents the corresponding (Re_t, Da_{H_2O}) combustion
 509 diagram. It shows that the obtained supersonic combustion regimes lie below
 510 the zone delineated by Ingenito and Bruno [76]. This result is fully consistent
 511 with the study of Cock [120] who scrutinized the effects (on Damköhler
 512 number estimates) of a multi-step finite-rate chemical kinetics description
 513 compared to a single-step chemistry. The large gap, of about two decades,
 514 that is observed between the present set of results and those documented in
 515 reference [76], is thus ascribed to the use of a finite-rate multi-step chemistry.

516 Moreover, the present set of results lies in the vicinity of the low boundary
 517 (*i.e.*, minimum bounds in Re_t and Da_{H_2O}) of the possible domain defined by
 518 Balakrishnan and Williams [75], which is depicted in blue color in Fig. 14.
 519 At this level, it is noteworthy that, as emphasized by Balakrishnan and
 520 Williams, the main effect of heat release is to reduce the turbulent kinetic
 521 energy, an effect that has not been considered in the delineation of the cor-
 522 responding domain in reference [75]. The work of Cock [120] and the more
 523 recent analysis of Fureby [121] also documented the way the heat release
 524 may alter the turbulence intensity in high-speed flow conditions. The results
 525 of reference [121] feature very large compressibility effects, with turbulent
 526 Mach number values of the order of 1.5 while the turbulent Reynolds num-
 527 ber values lie between 10^2 and 10^4 . In the present conditions, a decrease in
 528 the turbulence intensity from ten to five percent is observed across the reac-
 529 tive zone. This is in good agreement with the observations made by Ingenito
 530 and Bruno [76] but it should be however emphasized that larger turbulence
 531 intensity can be expected in confined conditions.

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

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

552 The diagram displayed in Fig. 15(a) shows that the points where the
553 probability to lie within a premixed combustion zone is the most important
554 are gathered around the isoline $Da_L = 1.0$ and lie within the broken flamelets
555 regime, which can be associated to thickened-wrinkled flame regime in the
556 Barrère-Borghini coordinates. This region is also characterized by supersonic
557 flow conditions (*i.e.*, $Ma > 1.0$). In this respect, the combustion diagram
558 reported in Fig. 15(c) also indicates that the sonic line follows closely the
559 low limit of the supersonic combustion regimes delineated by Ingenito and
560 Bruno [76]. As pointed out by Balakrishnan and Williams [75], this dia-
561 gram does not incorporate neither the compressibility nor the high-Mach num-
562 ber effects, which can be important in high-speed flow conditions. Thus,
563 the turbulent Mach number, which provides a measure of compressibility
564 effects on turbulence, has been also considered. Its value is significant (be-
565 tween 0.2-0.3) in regions where the heat release rate is highest, *i.e.*, in the
566 vicinity of the wall ($y/D < 1.0$), then it decreases in the regions that are
567 associated to the broken flamelet regime. At this level, it is noteworthy that
568 Fureby [121] has conducted a similar analysis on the HyShot II configura-
569 tion. In this study important compressibility effects were put into evidence,
570 with turbulent Mach number values that can be locally as high as 1.5. The
571 corresponding regions are under the influence by the counter-rotating vor-
572 tices pair (CVP), shock reflection, and shock-induced ignition. Indeed, in
573 the simulated geometry, the shock train certainly allows for the persistence
574 of a high level of velocity fluctuations at each reflected shock wave crossing.
575 Finally, the last two diagrams reported in Figs. 15(e) and 15(f) display the
576 scatterplots colored by the normalized coordinates and thus allow to identify
577 the flow regions in which the various turbulent combustion regimes develop.
578 In the near wall region and in the vicinity of the injection port, the com-
579 bustion regime is mostly that of a PSR, while farther from the wall and
580 hydrogen injection, the broken flamelets regime is the most probable.

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

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

612 The inspection of the Mach number shows that the fast chemistry regimes
 613 ($1.0 < Da_i < 100.0$) are relevant to supersonic flow conditions ($Ma > 1.2$).
 614 The turbulent Mach number values indicate that the compressibility effects
 615 are important in the near wall region $y/D < 1.0$, *i.e.*, in regions featuring
 616 significant heat release rates.

617 5. Conclusions and prospects

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

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

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

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

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

705

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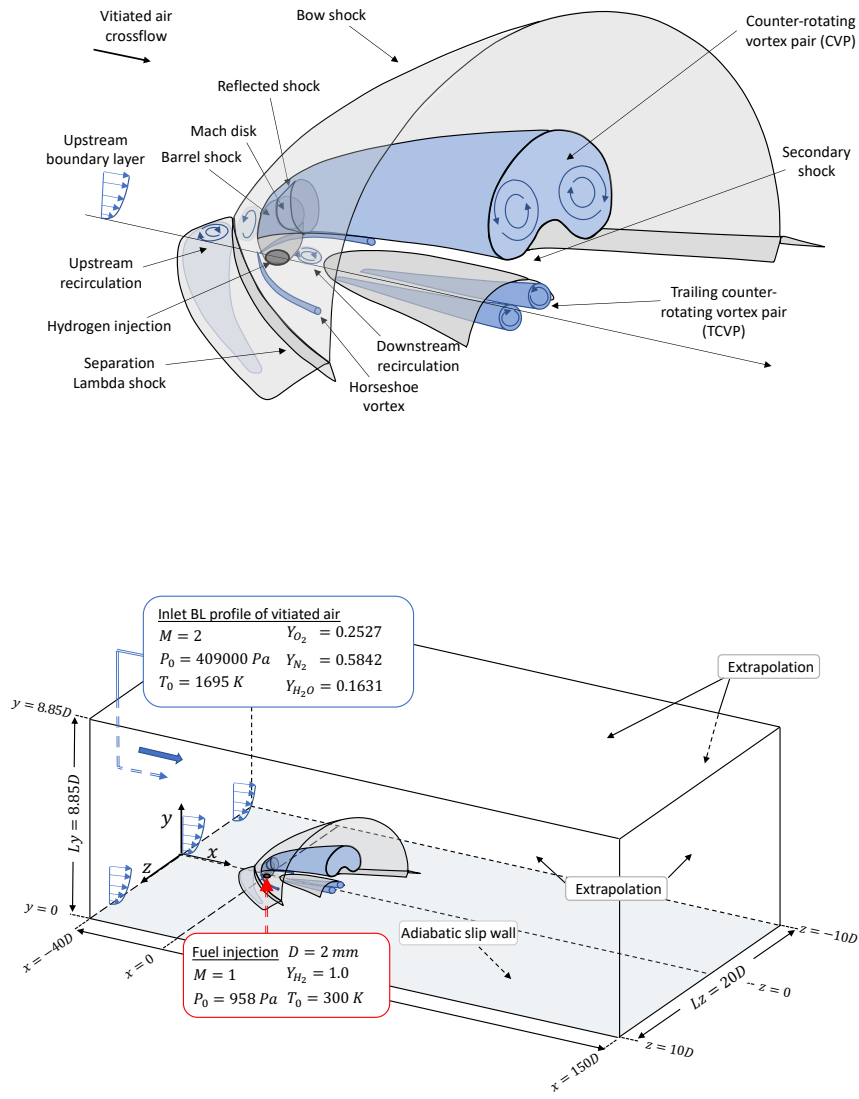


Fig. 1. Top: three-dimensional schematic view of the flow topology of the underexpanded jet in supersonic crossflow (JISCF). Bottom: definition of the computational domain and associated boundary conditions.

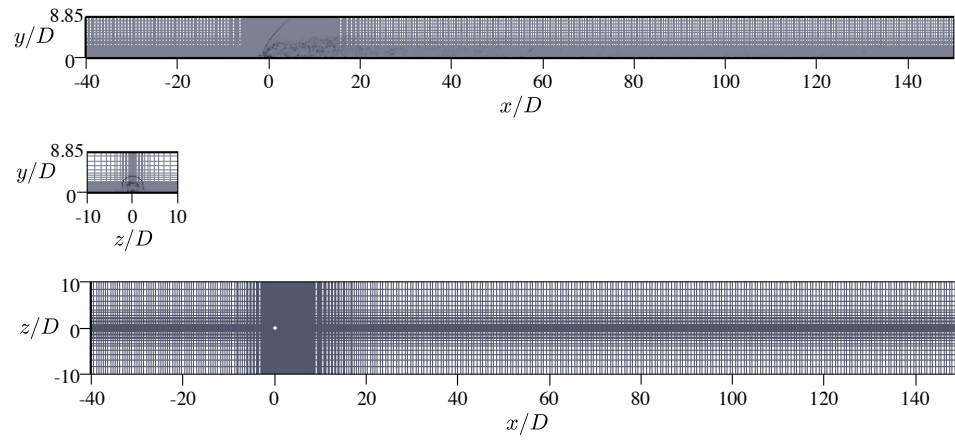


Fig. 2. Computational mesh overview (one single line depicted for six successive nodes).

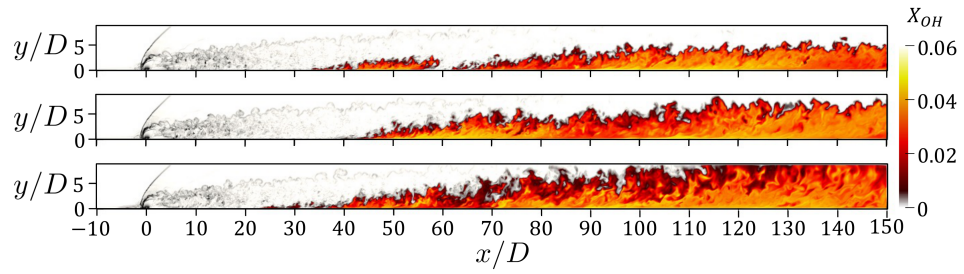


Fig. 3. Temporal evolution in the median plane $z/D = 0.0$ of the molar fraction of hydroxyl radical displayed together with a numerical Schlieren, from top to bottom, $t^* = 80.0$, 100.0 , and 170.0 .

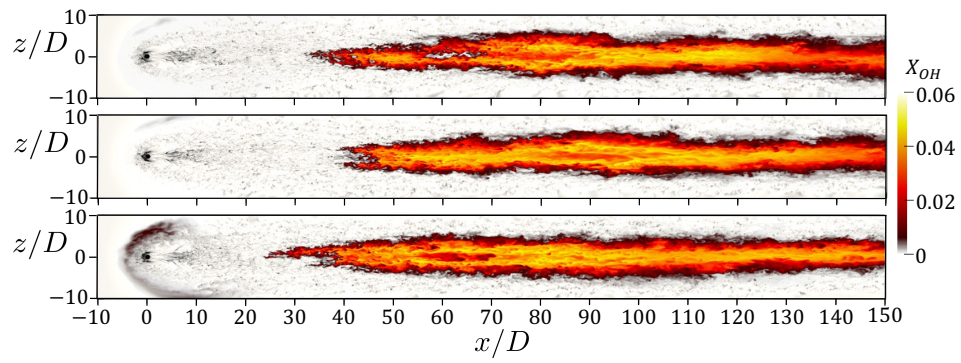


Fig. 4. Temporal evolution in the median plane $y/D = 0.25$ of the molar fraction of hydroxyl radical displayed together with a numerical Schlieren, from top to bottom, $t^* = 80.0$, 100.0 , and 170.0 .

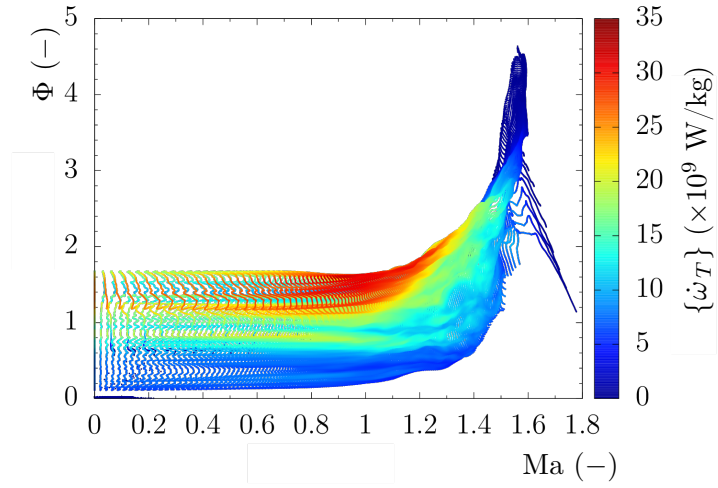


Fig. 5. Distribution of the combustion regime (subsonic / supersonic) evaluated in conditions featuring a HRR value that exceeds one percent of its maximal value $\dot{\omega}_{T,\max}$. The equivalence ratio is plotted versus the Mach number and the distribution is colored by the averaged HRR.

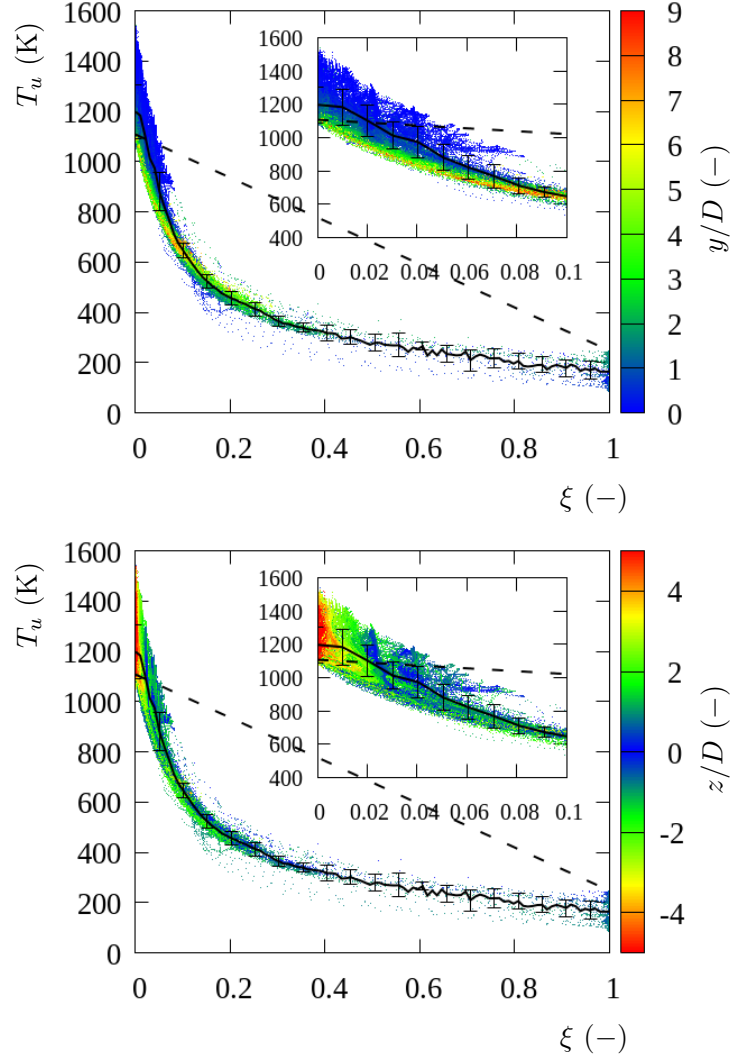


Fig. 6. Scatterplots of the unburnt mixture temperature obtained at $t = t_i = 150.0D/u_\infty$ plotted versus the mixture fraction as extracted from planes $x/D = 0.0, 25.0, 50.0,$ and 100.0 together with the corresponding conditional average (continuous black line) and with the linear approximation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

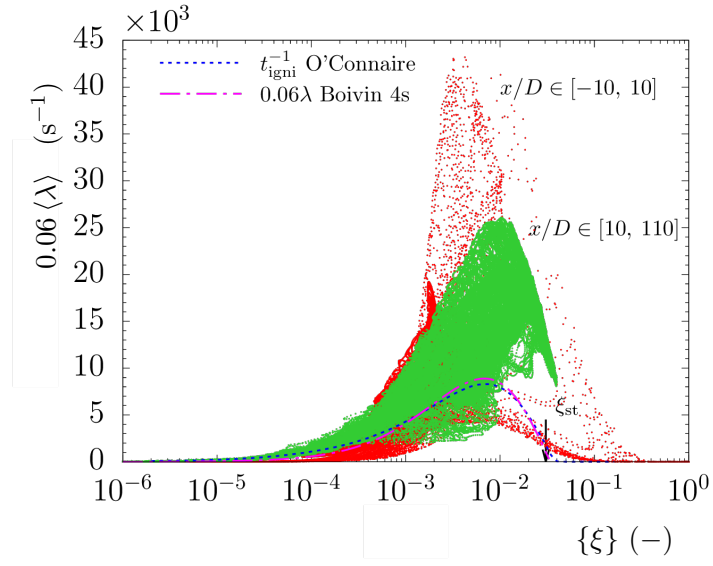


Fig. 7. Scatterplots of the reactivity λ plotted versus the mixture fraction in the direct vicinity of the injection ($-10.0 < x/D < 10.0$; red dots) and downstream of the injection ($10.0 < x/D < 110.0$; green dots). Comparison between PSR computations of (i) the ignition delay using the chemical scheme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

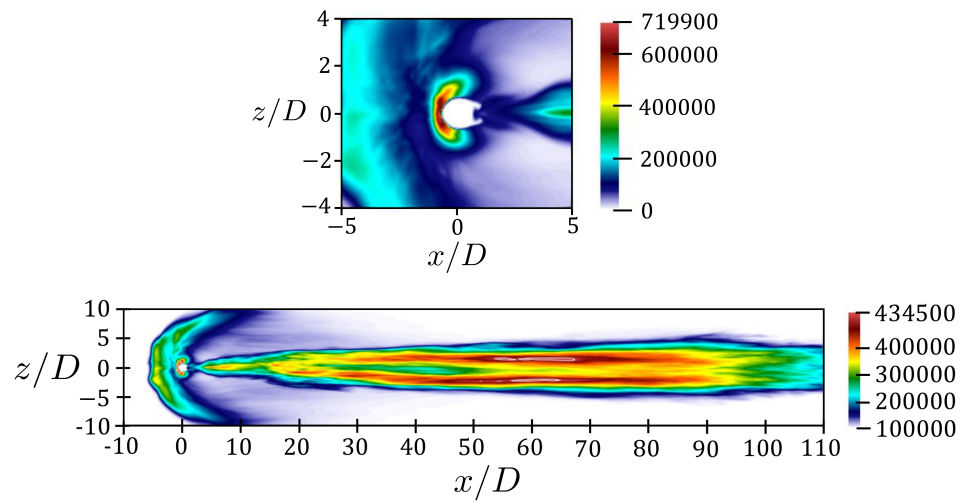


Fig. 8. Parietal field of the averaged reactivity $\langle \lambda \rangle$ (s^{-1}). Zoom on the injection (top) and general view (bottom). The isoline $0.95 \langle \lambda \rangle_{\max}$ is depicted with a white line.

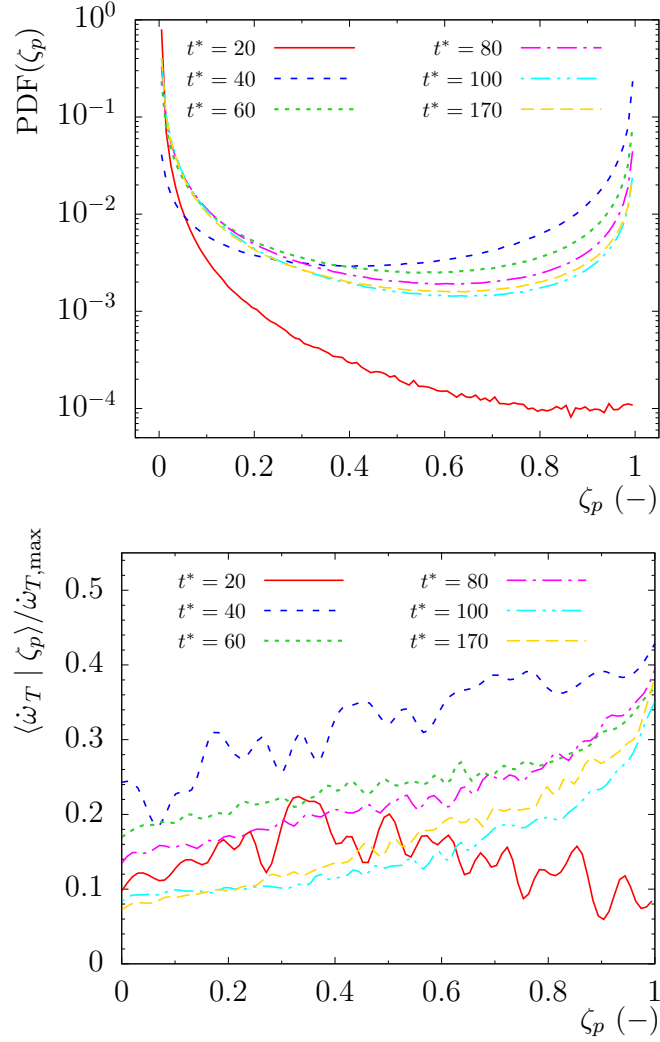


Fig. 9. Analysis of the non-premixed and premixed modes contributions evaluated in computational cells featuring a HRR value that exceeds one percent of its maximal value $\dot{\omega}_{T,\max}$ at times $t^* = 20.0, 40.0, 60.0, 80.0, 100.0,$ and 170.0 . Top: probability density function (PDF) of the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

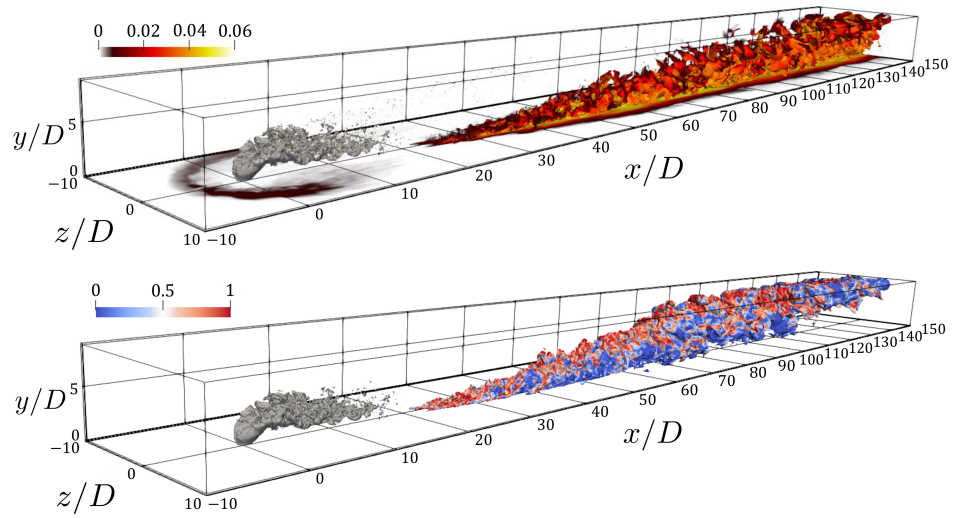


Fig. 10. Instantaneous flame structure at $t^* = 170.0$. Top: iso-surface of the stoichiometric mixture fraction colored by the OH molar fraction and parietal field of the same quantity. Bottom: iso-surface of the stoichiometric mixture fraction colored by the premixedness index. The grey iso-surface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

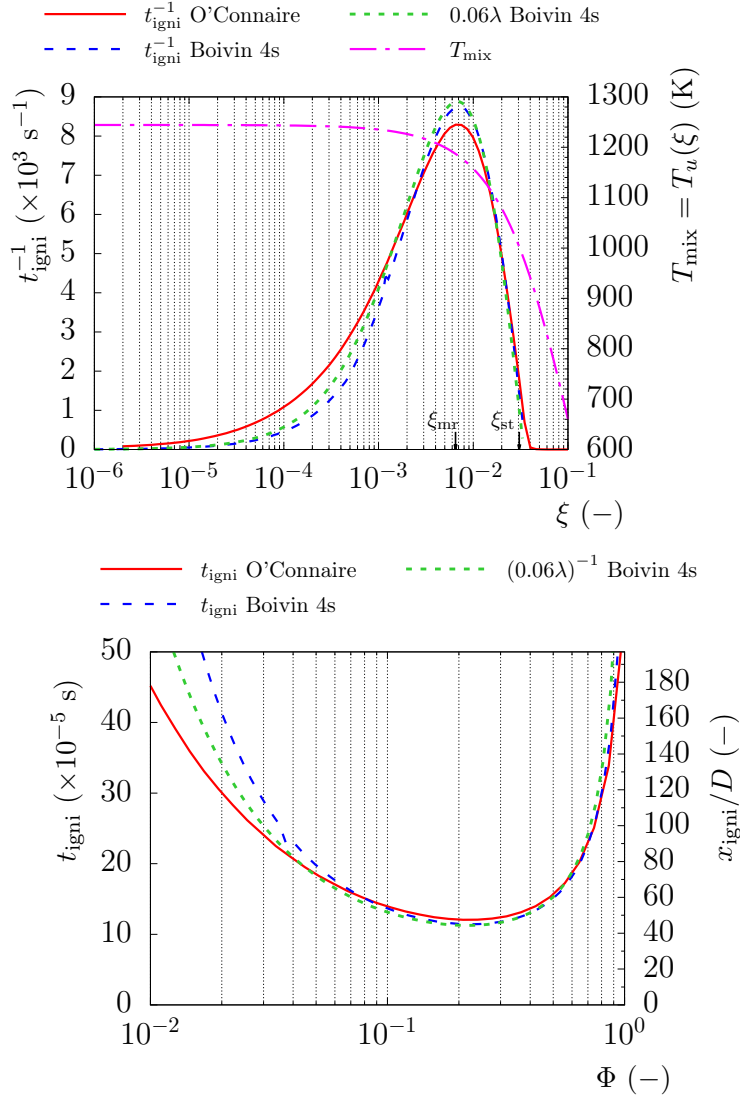


Fig. 11. Ignition delay time t_{igni} plotted versus the mixture fraction ξ (top) and equivalence ratio Φ (bottom) with a range of variation equivalent to $\xi \in [3.0 \cdot 10^{-4}, \xi_{\text{st}}]$. Comparison between the results obtained with the detailed mechanism of Ó Connaire *et al.* [102], 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 $x_{\text{igni}} = 0.6u_{\infty}t_{\text{igni}}$.

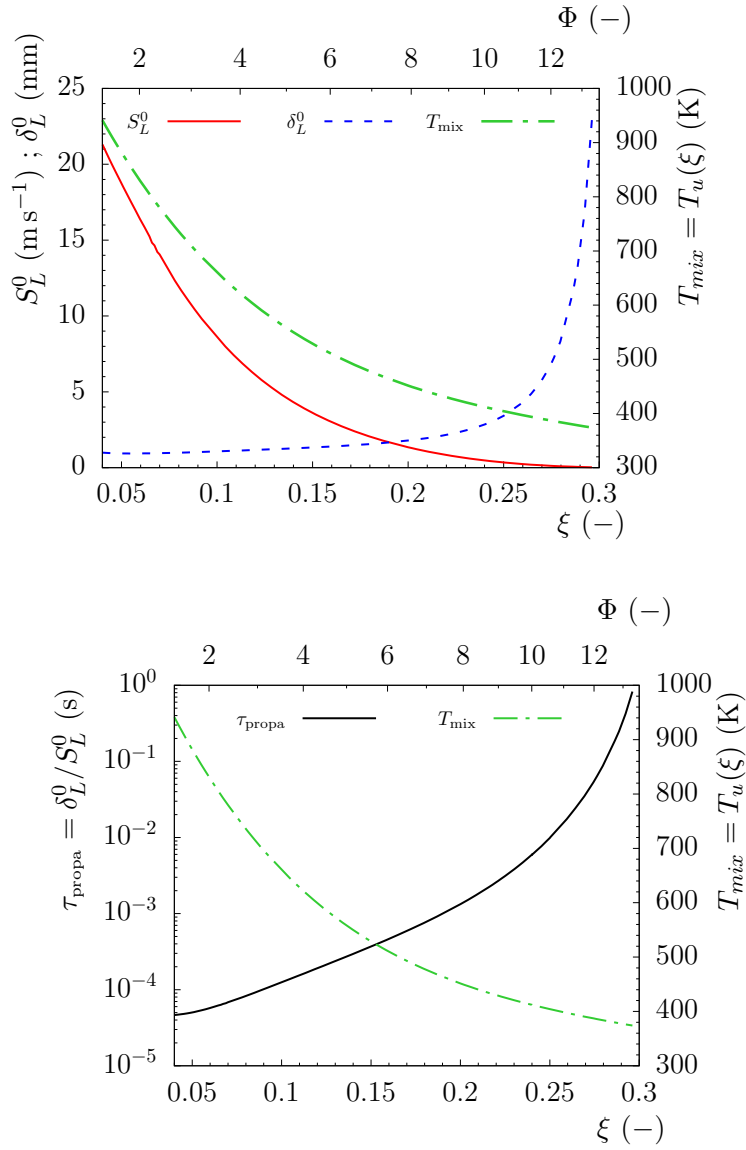


Fig. 12. Laminar flame velocity S_L^0 and thickness δ_L^0 (top) and flame transit time δ_L^0/S_L^0 (bottom) as a function of the mixture fraction ξ (and global equivalence ratio Φ). Computations performed with the detailed mechanism of Jachimowski *et al.* [110].

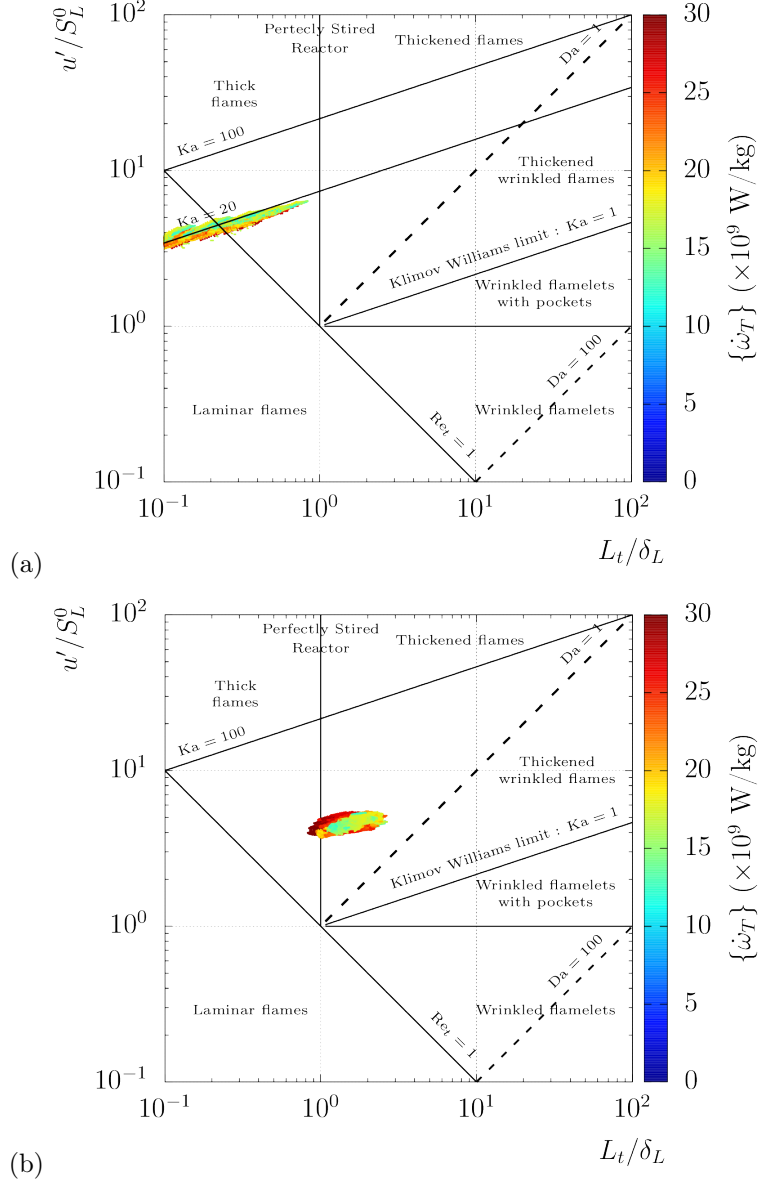


Fig. 13. Combustion regime scatterplots in the Barrère-Borghgi coordinates. Data are collected in plane $y/D = 0.0$ (Fig. 13(a)), in plane $y/D = 0.25$ (Fig. 13(b)), in the longitudinal median plane $z/D = 0.0$ (Fig. 13(c)), and in cross-stream planes $x/D = 25.0, 50.0, 75.0, 100.0,$ and 125.0 (Fig.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

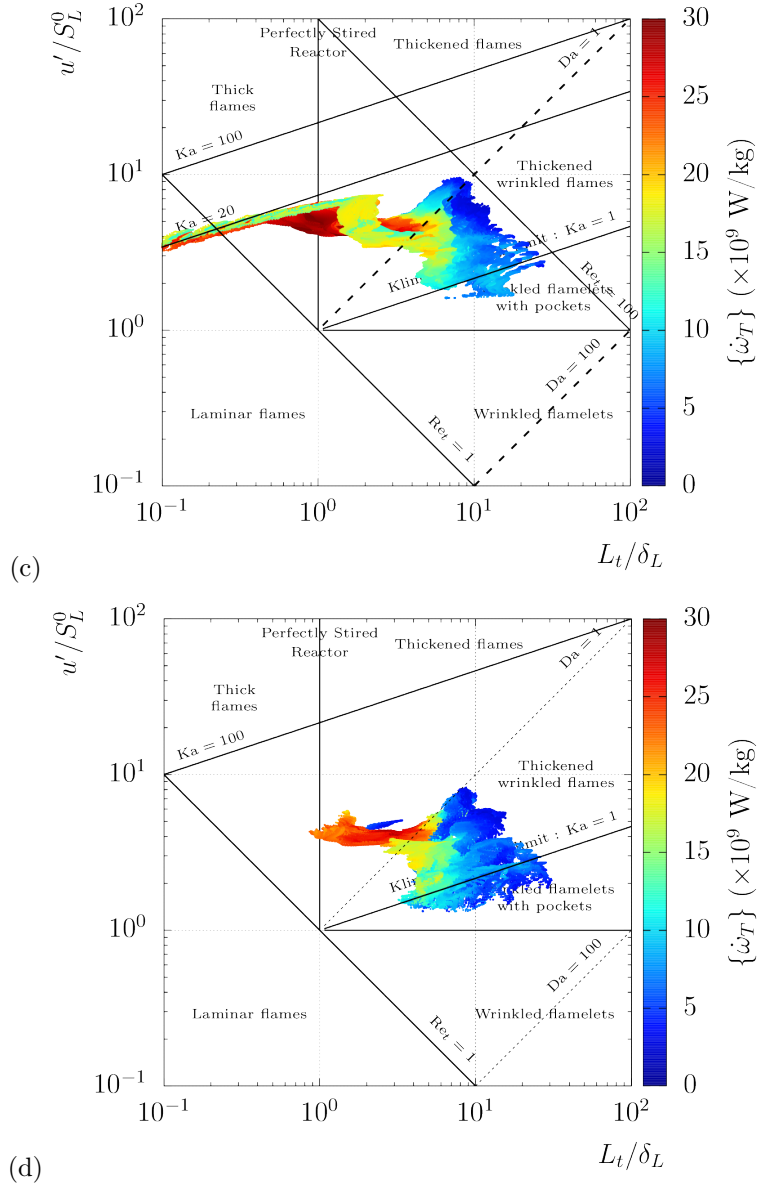


Fig. 13. Cont'd.

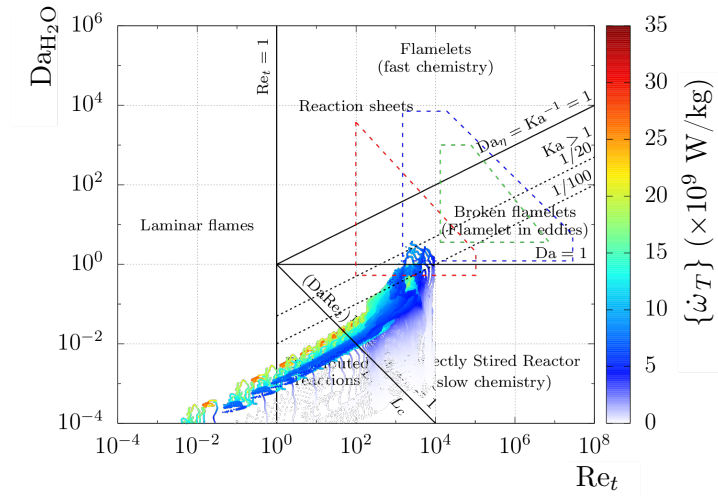


Fig. 14. Turbulent combustion diagram (Re_t, Da_{H_2O}) with a chemical time scale deduced from the water vapor production rate. Data are collected in the median plane ($z/D = 0.0$). Dots are colored by the heat release rate. The red frame corresponds to the supersonic combustion regimed defined by Ingenito and Bruno [76]. The blue and green frames stand for the possible and most probable domains introduced by Balakrishnan and Williams [75].

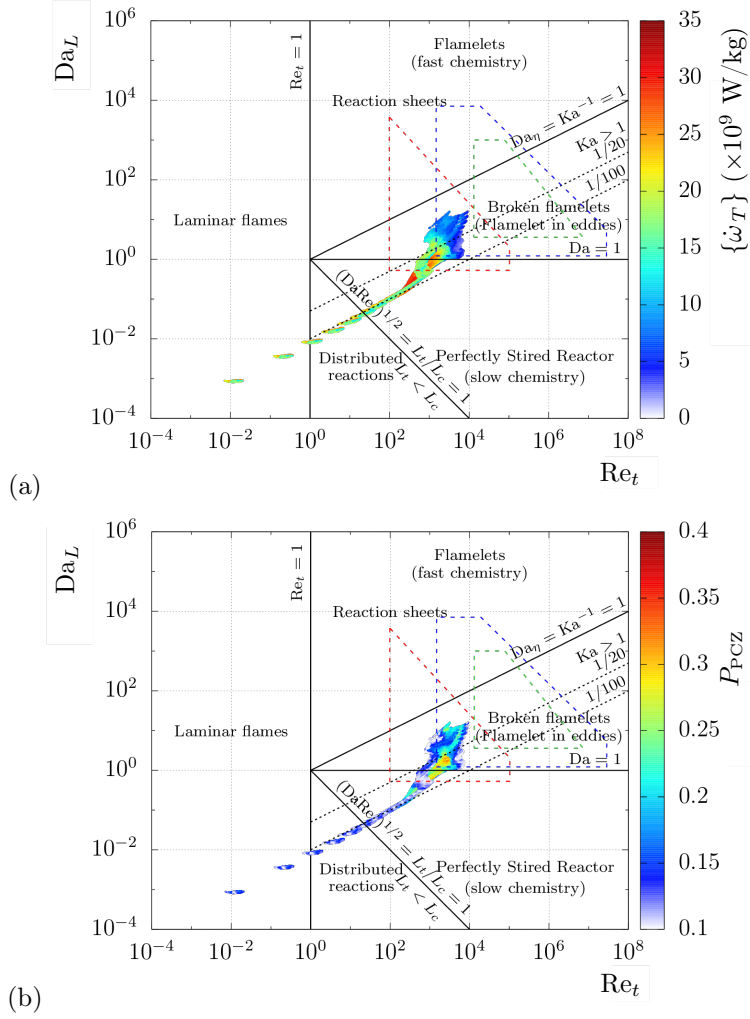
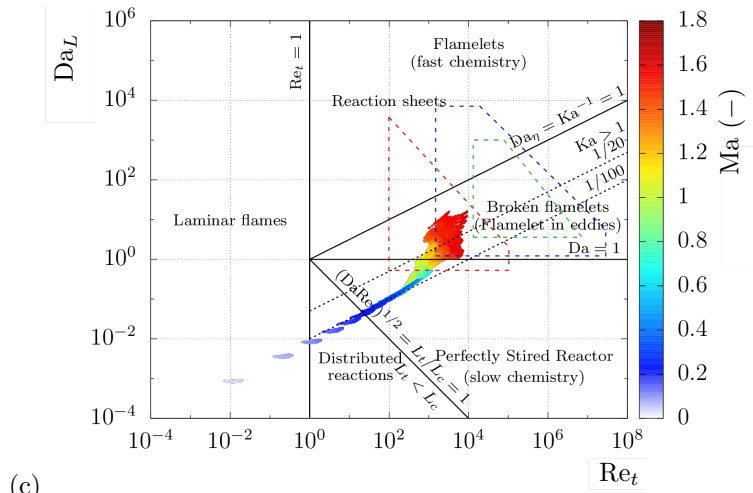
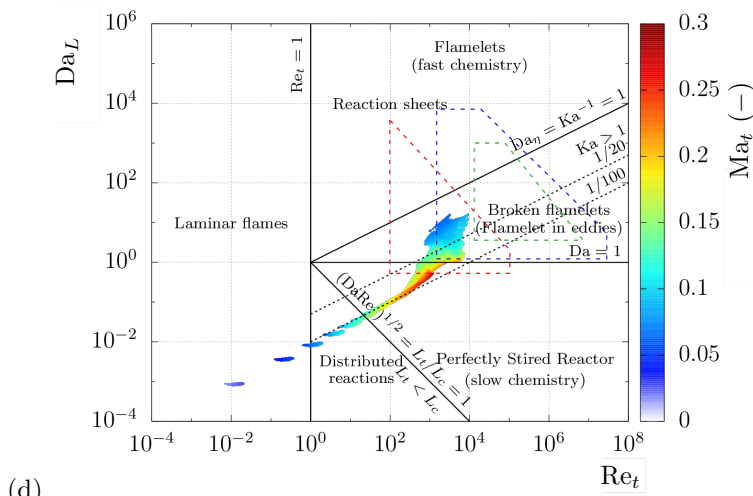


Fig. 15. Turbulent combustion diagrams (Re_t, Da_L) with a chemical time scale deduced from the laminar premixed flame transit time δ_L^0/S_L^0 . Data are collected in the median plane ($z/D = 0.0$). Dots are colored by (i) the heat release rate (Fig. 15(a)), (ii) probability that the premixedness index 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)).

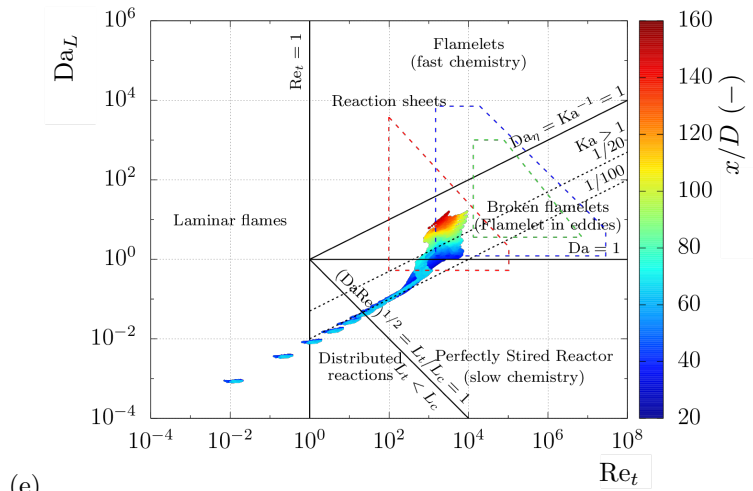


(c)

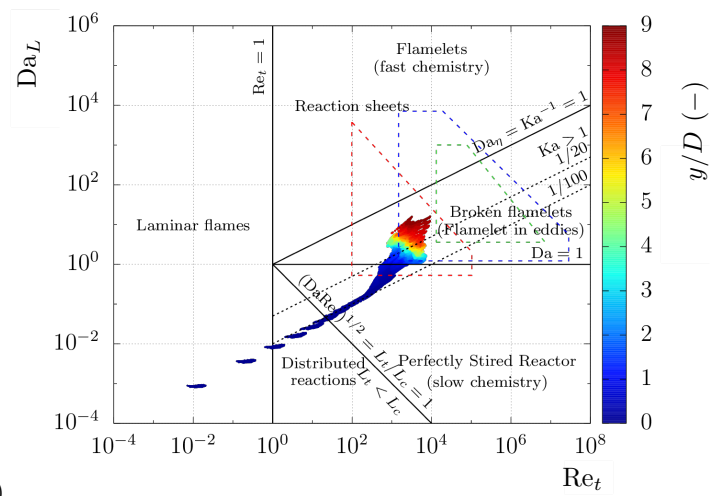


(d)

Fig. 15. Cont'd.



(e)



(f)

Fig. 15. Cont'd.

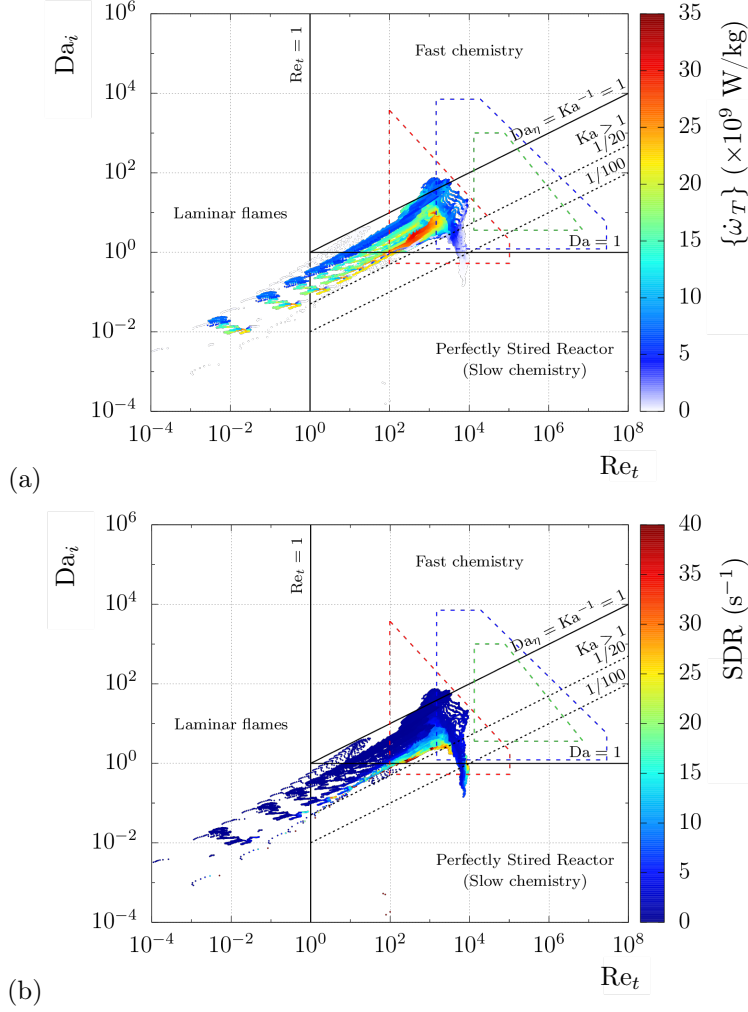
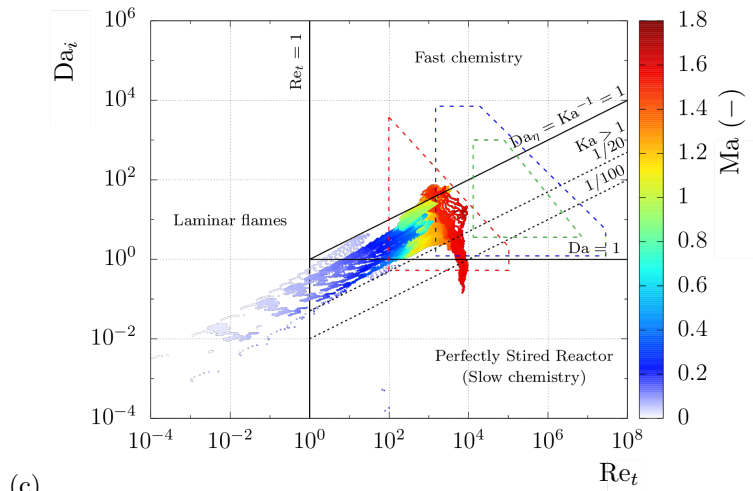
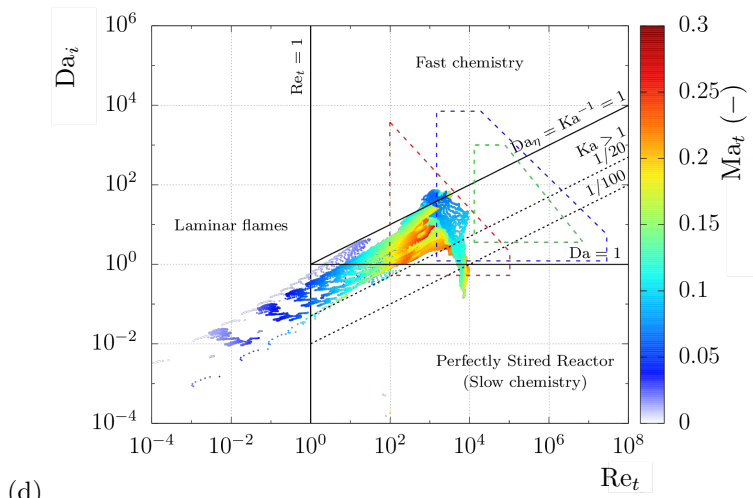


Fig. 16. Turbulent combustion diagrams (Re_t, Da_i) with a chemical time scale deduced from the reactivity λ . Data are collected in the median plane ($z/D = 0.0$). Dots are colored by (i) the heat release rate (Fig. 16(a)), (ii) the SDR (Fig. 16(b)), (iii) Mach number Ma (Fig. 16(c)), (iv) turbulent 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)).



(c)



(d)

Fig. 16. Cont'd.

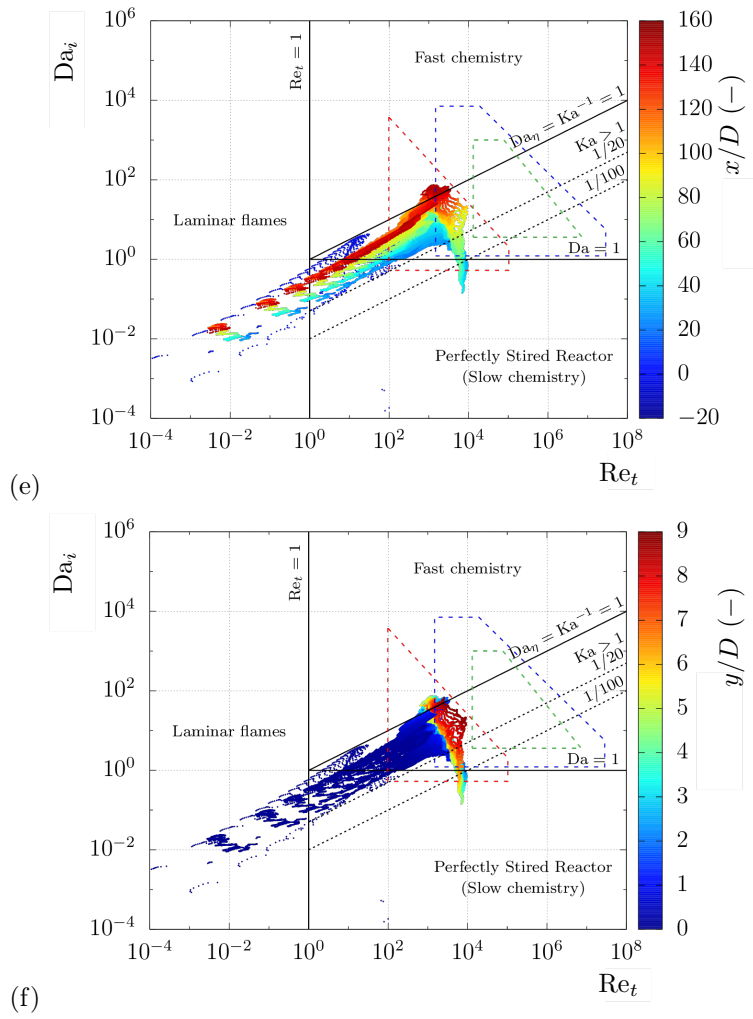


Fig. 16. Cont'd.