1 Influence of synthetic inlet turbulence
2 on the prediction of low Mach number flows

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17 **Abstract**

Time-resolved numerical simulations of fluid flows, such as Large Eddy Simulations (LES), have the capability of simulating the unsteady dynamics of large scale energetic structures. However, they are known to be intrinsically sensitive to inflow conditions the modelling of which may become a crucial ingredient of the computational model. The present work reports LES of both reactive and non-reactive turbulent channel flows. The flow configuration and associated conditions correspond to those associated with a reference experimental database that has been gathered at the French aerospace Laboratory of Onera. The focus of our study is placed on the influence of synthetic inlet turbulence in this experimental geometry, i.e., the principal aim is to investigate the sensitivity of the flow dynamics and mixing to inflow conditions. The analysis undoubtedly confirms that, even with properly set mean velocity and turbulence kinetic en-

ergy profiles as available from experimental data, both non-reactive and reactive flow fields still remain very sensitive to the choice of the synthetic turbulence model. This sensitivity is illustrated for four distinct turbulent inflows obtained from *white noise* (WN), *digital filter* (DF) by Klein et al. (2003), *random flow generator* (RFG) by Smirnov et al. (2001), and *synthetic eddy model* (SEM) by Jarrin et al. (2009). Finally the results obtained for reactive flow conditions clearly emphasize the influence of the retained model on the chemical reaction rate statistics. This conclusion confirms how relevant are the developments devoted to synthetic turbulence for the computational investigation of turbulent combustion.

18 *Keywords:* Turbulent inflow boundary conditions, Large Eddy Simulation,
 19 Synthetic inlet turbulence, Low Mach number flows, Reactive flows

20 **1. Introduction**

21 It is well known that a subject of great importance for fluid flow numerical
 22 simulations is the prescription of correct and realistic boundary conditions. For
 23 outflow conditions, it appears that the use of a buffer zone (Bodony, 2006) or
 24 an advective boundary condition (Orlanski, 1976), or even a combination of
 25 both, may adequately describe several flow conditions of practical interest. The
 26 present work is focused on low Mach number flows and the main difficulty is thus
 27 concentrated on the settlement of the inlet velocity field. In contrast, for com-
 28 pressible flows, specifying the fourth variable (pressure, density, temperature or
 29 characteristic wave) may also become a critical issue which raises a wide range of
 30 additional specific difficulties. In such conditions, elaborate strategies should be
 31 used to avoid pressure wave reflections, see for instance Rudy and Strikwerda
 32 (1980); Thompson (1987); Poinso and Lele (1992); Albin et al. (2011). The
 33 specification of inflow boundary conditions may also raise several issues. Most
 34 flows encountered in real applications are, indeed, spatially developing turbulent
 35 flows. Hence, they pose a great challenge for numerical simulations due to the

36 need to prescribe time-dependent turbulent inflow data at the upstream bound-
 37 ary. For steady Reynolds-Averaged Navier-Stokes (RANS) simulations, simple
 38 analytical or experimental profiles are retained for mean velocity components
 39 and turbulent characteristics. For LES or Direct Numerical Simulations (DNS),
 40 however, the inflow data should consist of an unsteady fluctuating velocity sig-
 41 nal representative of the turbulent velocity field at the inlet.

42 A basic technique to generate such a turbulent inflow data consists in taking
 43 a mean velocity profile with superimposed random noise. The major drawback
 44 of such a methodology is that the resulting inflow data do not exhibit any spatial
 45 and/or temporal correlations. The energy generated is, also, uniformly spread
 46 over all wave numbers and, due to the lack of large scale energy-containing
 47 structures, *turbulence* is quickly dissipated (Jarrin et al., 2009).

48 In principle it may be possible to predict turbulence via a LES technique
 49 by starting from a quiescent flow or with the mean flow field obtained from
 50 RANS simulations. Unfortunately, a very long time is required for a turbulent
 51 flow to spatially and temporally develop (Smirnov et al., 2001). Ideally, the
 52 simulation of the upstream flow entering a computational domain would pro-
 53 vide realistic inlet conditions to the simulation of interest. However, due to the
 54 computational cost, the domain cannot be extended upstream indefinitely, and
 55 approximate turbulent inlet conditions must therefore be specified.

56 There are several ways to remedy this situation, and the existing methods
 57 belong to two principal categories: *(i) mapping or recycling methods*, in which
 58 some sort of turbulent flow is pre-computed, prior to the main calculation,
 59 and subsequently introduced at the domain inlet, and *(ii) synthetic turbulence*
 60 *methods*, in which some form of random fluctuation is generated, modulated
 61 according to experimental data, and combined with mean inflow. Other appeal-
 62 ing strategies have been introduced in the literature, some of them are based on
 63 Fourier techniques, and others rely on the Proper Orthogonal Decomposition
 64 (POD) introduced by Lumley (1967), see for instance Druault et al. (2004).

65 The present manuscript is organized as follows: first a brief description of
 66 recycling methods is provided. Further, synthetic turbulence generators are pre-

67 sented, and the four methods considered in the present work are detailed: (i) the
 68 *white noise* (WN), (ii) the digital filter (DF) method proposed by Klein et al.
 69 (2003), (iii) the *Random Flow Generator* (RFG) introduced by Smirnov et al.
 70 (2001) and (iv) the *Synthetic Eddy Method* (SEM) of Jarrin et al. (2009). The
 71 synthetic turbulence generators have been implemented in a low Mach number
 72 Navier-Stokes solver, the main features of which are presented, including a brief
 73 description of both mathematical and numerical aspects. As a preliminary step
 74 of verification and validation, the methods are applied to the description of ho-
 75 mogeneous isotropic turbulence. The computational programs are then further
 76 assessed by analyzing their capabilities of generating a fluctuating signal which
 77 reproduces a given stress tensor and features an energy spectrum similar to
 78 the one associated with a fully developed turbulent flow spectrum. The former
 79 means that the inflow data generator should be able to reproduce an anisotropic
 80 turbulent velocity field at the inlet. The paper ends with the application of the
 81 above-mentioned synthetic turbulence generators to the numerical simulation of
 82 high speed non-reactive and reactive turbulent mixing layers, which were exper-
 83 imentally studied by Moreau and Boutier (1977), see also Magre et al. (1988).
 84 Comparisons with available experimental data are provided.

85 **2. Literature review**

86 The specification of realistic turbulent inflow boundary conditions remains
 87 a challenging issue for both LES and DNS. This is quite a contrast to RANS or
 88 URANS applications for which a scale separation argument is implied between
 89 the unsteadiness of the mean flow field and the associated turbulent fluctuations.
 90 The quantities being computed in RANS or URANS are thus steady or varying
 91 on a characteristic time scale that is much larger than the computational time
 92 step. Such a scale separation argument does not hold for DNS or LES which
 93 therefore require a special treatment of turbulent fluctuations at inlet conditions.
 94 A review of some of the existent methods that deal with the specification of such
 95 turbulent inflow conditions is provided below.

96 2.1. Mapping methods

97 The most accurate method to specify turbulent fluctuations for either LES or
98 DNS would probably consist in running a suitable precursor simulation with the
99 purpose of providing the main simulation with accurate boundary conditions.
100 However, such a procedure has been used only when the turbulence at the inlet
101 can be regarded as a fully developed or a spatially developing boundary layer.
102 In these cases periodic boundary conditions in the mean flow direction can be
103 applied to the precursor simulation. In general, the simulation of the precursor
104 flow is initialized with a mean velocity profile perturbed with a few unstable
105 Fourier modes. Instantaneous velocity fluctuations in a plane positioned at a
106 fixed streamwise location are extracted from the precursor simulation and pre-
107 scribed at the inlet of the main simulation at each time step.

108 In practice, periodic boundary conditions can only be used to generate inflow
109 conditions for homogeneous flows in the streamwise direction, which restricts
110 their applications to simple fully developed flows. A more flexible technique to
111 generate inlet conditions, also based on the procedure of recycling the velocities
112 in a plane located several boundary layer thicknesses downstream of the inlet,
113 has been proposed by Lund (1998). In this framework, the velocity field at the
114 re-scaling station is decomposed into mean and fluctuating components; scaling
115 is applied to the mean and to the fluctuating parts in the inner and outer lay-
116 ers to account for the different similarity laws that govern both regions. The
117 scaled velocity is then re-introduced as a boundary condition at the inlet of the
118 computational domain. The use of such a methodology results in a spatially
119 evolving boundary layer simulation that is capable of generating its own inflow
120 data.

121 Another strategy has been followed by Li et al. (2000) who proposed a pro-
122 cedure to reduce the storage requirement, as well as the computational cost
123 associated with a precursor calculation. A spatially developing turbulent mix-
124 ing layer, originating from the mixing of a low-speed and a high-speed boundary
125 layer flow at the end of a splitter plate, is simulated within the LES context.
126 However, instead of simulating the precursor boundary layer flow fields, only a

127 time series of instantaneous velocity planes with duration approximately equal
 128 to the integral time scale of the flow is extracted from a boundary layer sim-
 129 ulation. The resulting signal is converted into a periodic one using a classic
 130 windowing technique, and it is used, as many times as required, to obtain con-
 131 verged statistics in the main simulation. This methodology is beneficial from
 132 both the computational and storage points of view, since the precursor sim-
 133 ulation is run over a short duration only and the data used to generate the
 134 inflow correspond to a few integral time scales of the flow. For the investigated
 135 mixing layer simulation, the periodicity involved by the inflow decays rapidly,
 136 in approximately 25 per cent of the total length of the computational domain.
 137 However, Li et al. (2000) reported that the resort to this procedure for wall-
 138 bounded flows, where destabilizing effects remain relatively weak, might require
 139 a longer transition region to weaken the effects of the periodicity condition that
 140 is involved in the inflow prescription.

141 Finally, Bodony (2006) noted that the method introduced by Lund (1998),
 142 i.e., random uncorrelated fluctuations superimposed on a mean velocity profile,
 143 is very sensitive to the initialization of the flow field. Bodony (2006) also stated
 144 that the generation of fully developed turbulence cannot be obtained from such
 145 a strategy and, hence, proposed a more robust variant of the original method of
 146 Lund (1998), where the flow field is initialized thanks to synthetic turbulence
 147 with prescribed energy spectrum and shear stress profile.

148 To conclude it is noteworthy that other mapping techniques have been pro-
 149 posed in the context of hybrid RANS-LES simulations. For instance, Schlüter
 150 et al. (2004) fed the LES of a combustor with the Favre-averaged mean velocity
 151 field $\tilde{u}_i$ issued from a RANS solution together with a fluctuating component
 152 $u_i - \tilde{u}_i$. The latter is extracted from a database which was generated from
 153 an auxiliary LES computation and the corresponding turbulent fluctuations
 154 are rescaled to match mean and fluctuations statistics issued from the RANS
 155 simulation.

156 2.2. Synthetic turbulence generators

157 Methods that do not rely on a precursor simulation, or re-scaling of a
158 database obtained from a precursor simulation, synthesize inflow conditions
159 using some sort of stochastic procedure. These procedures use random number
160 generators to build a fluctuating velocity signal similar to those observed in
161 turbulent flows. This is possible based on the assumption that a turbulent flow
162 can be approximated from a set of low order statistics, such as mean velocity,
163 turbulent kinetic energy, Reynolds stresses, two-point or two-time correlations.
164 However, it is worth emphasizing that the resulting synthesized signals remain
165 only a crude approximation of turbulence. From a statistical point of view,
166 some crucial quantities, such as the dissipation rate, the turbulent transport or
167 the pressure-strain term that appear in the Reynolds stresses balance are often
168 not well reproduced. The dynamics of the turbulent eddies are not perfectly
169 recovered, and the synthesized flow may undergo a transition to turbulence.
170 Therefore, synthesized turbulence can have a structure that significantly differs
171 from that of the real flow fields (Jarrin et al., 2009).

172 2.2.1. White noise based synthetic turbulence generators - WN

173 The most straightforward approach to build synthetic fluctuations is to gen-
174 erate a set of independent random numbers between zero and unity which can
175 *mimic* the turbulence intensity at the inlet. Indeed, if the turbulent kinetic
176 energy level k is known, it can be used to scale a random signal $\mathcal{R}_{u_i}$ with zero
177 mean and unity variance. Thus, the fluctuations exhibit the correct level of
178 turbulent kinetic energy, which yields $u_i = \tilde{u}_i + \mathcal{R}_{u_i} \sqrt{2k/3}$, where $\mathcal{R}_{u_i}$ is taken
179 from independent random variables for each velocity component at each instant
180 and location on the computational inlet plane. This procedure generates an
181 isotropic random signal that reproduces both the mean velocity and turbulent
182 kinetic energy levels. However, the signal generated does not present any two-
183 point nor two-time correlations.

184

185 If the Reynolds stresses tensor (R_{ij}) is available, Lund (1998) introduced the

186 following transformation rule to reconstruct correlated velocity components:

$$u_i = \tilde{u}_i + \mathcal{R}_{u_j} a_{ij}, \quad (1)$$

187 where (a_{ij}) denotes the Cholesky decomposition of the symmetric positive de-
188 fined Reynolds stress tensor (R_{ij}) ,

$$a_{ij} = \begin{pmatrix} \sqrt{R_{11}} & 0 & 0 \\ R_{21}/a_{11} & \sqrt{R_{22} - a_{21}^2} & 0 \\ R_{31}/a_{11} & (R_{32} - a_{21}a_{31})/a_{22} & \sqrt{R_{33} - a_{31}^2 - a_{32}^2} \end{pmatrix}. \quad (2)$$

189 This strategy allows the basic random procedure to reproduce the targeted
190 cross-correlations between velocity components.

191 Although the methods presented above are capable of reproducing some
192 characteristics of real turbulent flow fields, such as the anisotropy, they do not
193 account for any correlations in either time or space. Therefore, these random
194 fluctuations have their energy spectrum uniformly spread over all wave numbers
195 and, as already stated above, this energy will be quickly dissipated downstream
196 of the inlet boundary. A more valuable approach for generating synthetic tur-
197 bulence therefore consists in creating bins of random data, which can then be
198 processed using digital filters, so that the resulting set of processed data will
199 display desired statistical properties, such as spatial and temporal correlations
200 (Lund, 1998; Klein et al., 2003).

201 2.2.2. Digital filters based synthetic turbulence generators - DF

202 Klein et al. (2003) proposed a digital filtering (DF) procedure to remedy the
203 lack of large-scale correlation in the inflow data generated through the above
204 method. In one dimension the fluctuating velocity signal u'_m at a point m is
205 defined as a convolution or a digital linear non-recursive filtering:

$$u'_m = \sum_{n=-M}^{n=M} b_n \mathcal{R}_{m+n}, \quad (3)$$

206 where $\mathcal{R}_m$ is a series of random data generated at point m with $\overline{\mathcal{R}_m} = 0$,
207 $\overline{\mathcal{R}_m \mathcal{R}_m} = 1$, $\overline{\mathcal{R}_m \mathcal{R}_n} = 0$ for $m \neq n$, and b_n are the filter coefficients. In the

previous expressions, the overbar denotes averaged values obtained from the series of random data. Note that, since the ergodic hypothesis is implied, the time average of one sequence of events is the same as the ensemble average. The integer number M is related to the size of the filter support. The relation between the filter coefficients and the two-point velocity correlation function is given by:

$$\frac{\sum_{j=-M+k}^{j=M} b_j b_{j-k}}{\sum_{j=-M}^{j=M} b_j^2} = \frac{\overline{u'_m u'_{m+k}}}{\overline{u'_m u'_m}} \quad (4)$$

This procedure is extended to the time-dependent generation of synthetic velocity field on a plane (Ox_2x_3) by generating a three-dimensional random field $\mathcal{R}_m(i, j, k)$ for each velocity component m . The indices i , j , and k are associated to the x_1 -direction (or time t by making use of the Taylor hypothesis), the x_2 -direction and the x_3 -direction, respectively. A three-dimensional filter $b(i, j, k)$ is obtained by the convolution of three one-dimensional filters: $b(i, j, k) = b_i \times b_j \times b_k$, in such a manner that the random data $\mathcal{R}_m(i, j, k)$ are filtered in the three directions x_1 , x_2 and x_3 ,

$$\mathcal{U}_m(j, k) = \sum_{i'=-M_{x_1}}^{i'=M_{x_1}} \sum_{j'=-M_{x_2}}^{j'=M_{x_2}} \sum_{k'=-M_{x_3}}^{k'=M_{x_3}} b_{i'} \times b_{j'} \times b_{k'} \mathcal{R}_m(i', j + j', k + k') \quad (5)$$

where j and k denote the location of the computational cell at the inlet plane, i.e., $j = 1, \dots, N_{x_2}$ and $k = 1, \dots, N_{x_3}$. Note that, in the following, we will retain an homogeneous filter width N in the three spatial directions, i.e., $M_{x_1} = M_{x_2} = M_{x_3} = N$.

In order to generate fluctuations that reproduce exactly the targeted two-point correlations, the filter coefficients b_k should be computed by inverting Eq. (4). However, since the two-point autocorrelation tensor is seldom available, Klein et al. (2003) assumed a Gaussian shape depending on one single parameter, the length scale $L = n\Delta x$ (N being such that $N \geq 2n$). The coefficients can then be computed analytically, without the cost of inverting Eq. (4), $b_p \approx$

233 $\hat{b}_p / \sqrt{\left(\sum_{j=-N}^{j=N} \hat{b}_j^2\right)}$ where $\hat{b}_j := \exp(-\pi j^2 / 2n^2)$. Once the processed random
 234 signal is evaluated by using Eq. (5), the final inflow velocity can be written as,
 235 $u_i = \tilde{u}_i + a_{im} \mathcal{U}_m(j, k)$ thanks to the Cholesky decomposition a_{ij} of the Reynolds
 236 stress tensor R_{ij} .

237 Following Klein et al. (2003), it is possible to generate a large amount of data,
 238 store and convect it through the inflow plane by applying Taylor's hypothesis.
 239 However, for the applications considered here, the inflow data will be generated
 240 on-the-fly. The implementation of the DF synthetic turbulence generator is
 241 indeed quite efficient and, for the present application, the computational costs
 242 associated to the database lookup technique were found greater than the online
 243 generation of the data. We therefore preferred to resort to the latter.

244 It should be noted that the main parameters retained to evaluate this method
 245 are the choice of the length scales, which are directly connected to the DF
 246 support size, and the dimensions of the control volume. Thus, a given value
 247 of the characteristic length scale may be reproduced by correctly choosing the
 248 filter support size as well as the control volumes dimensions. However, as will
 249 be shown below, the length scales and, consequently, the filter support size
 250 strongly impact on the computational cost of the method. Finally, since a
 251 fixed computational grid is used here to assess the different turbulent inflow
 252 generators, the parameters retained to evaluate the DF method will be the
 253 support size, only.

254 2.2.3. *Synthetic turbulence generators based on Fourier techniques - RFG*

255 In their recent review, Tabor and Baba-Ahmadi (2010) concluded that, since
 256 turbulence is often analyzed on the basis of a harmonic functions decomposi-
 257 tion, i.e., Fourier analysis, the fluctuations can be more efficiently represented
 258 by resorting to a linear sum of trigonometric functions, with the coefficients
 259 representing the energy contained in each mode.

260 To the authors best knowledge, Kraichnan (1970) was the first to use a
 261 Fourier decomposition to generate a synthetic fluctuating turbulent flow field.
 262 In Kraichnan's early work, the flow is initialized with a three-dimensional homo-

263 geneous and isotropic synthetic velocity field to study the diffusion of a passive
 264 scalar. Since the velocity fluctuations are homogeneous in the three dimen-
 265 sions, they can be decomposed in the Fourier space, $\mathbf{u}'(\mathbf{x}) = \sum_{\mathbf{k}} \hat{\mathbf{u}}'_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}}$,
 266 where $\mathbf{k}$ is a three-dimensional wave number vector. Each complex Fourier
 267 coefficient $\hat{\mathbf{u}}'_{\mathbf{k}}$ defines an amplitude evaluated from a prescribed isotropic three-
 268 dimensional energy spectrum $E(|\mathbf{k}|)$ and a random phase $\theta_{\mathbf{k}}$, taken uniformly in
 269 the $[0, 2\pi]$ interval (Rogallo, 1981). The synthesized velocity field is thus given
 270 by $\mathbf{u}'(\mathbf{x}) = \sum_{\mathbf{k}} \sqrt{E(|\mathbf{k}|)} e^{-i(\mathbf{k}\cdot\mathbf{x} + \theta_{\mathbf{k}})}$. Several adaptations of Kraichnan's method
 271 were proposed throughout the years. Among them, Lee et al. (1992) proposed
 272 one that allows for the application of Kraichnan's method to spatially evolving
 273 turbulent flows. They showed that it is possible to generate a synthesized tur-
 274 bulent time-evolving signal, in which the prescription of a phase shift between
 275 different time steps allows to obtain a synthesized velocity field at the inlet
 276 featuring correct temporal correlations. One remarkable advantage of such a
 277 method is that the generation of the turbulent signal can be performed by using
 278 *Fast Fourier Transform - FFT* algorithms, which are computationally very effi-
 279 cient. The capability of generating an anisotropic random signal was introduced
 280 by Le et al. (1997). Based on the method of Lee et al. (1992), an isotropic tur-
 281 bulent synthesized signal is generated and then re-scaled using Eq.(2). In this
 282 way the reconstructed fluctuations match a prescribed Reynolds stress tensor.
 283 However, if one is interested in initializing the whole computational domain, the
 284 method may present some limitations. Indeed, since it is based on direct and
 285 inverse transforms using FFT algorithms, its application to non-uniform grids
 286 is possible at the inlet plane only, which considerably reduces its interest for
 287 practical applications.

288 More recently, Smirnov et al. (2001) modified the method of Le et al. (1997)
 289 in such a manner that it becomes possible to obtain a turbulent velocity field
 290 by requiring statistical information only. The method of Smirnov et al. (2001)
 291 is capable of synthesizing non-homogeneous turbulence within a general frame-
 292 work. It relies on the Fourier decomposition, with Fourier coefficients computed
 293 from spectral data based on local turbulent time and length scales obtained at

different locations across the flow. This method, called *Random Flow Generation* and denoted RFG hereafter, differs from the original proposal of Lee et al. (1992) since it does not make use of Fourier transforms. It is based on scaling and coordinates transformation operations only, which, on non-uniform grids, are much more efficient.

The RFG computational routines used here are detailed in Smirnov (2004) and a brief description of the procedure retained to generate the turbulent inflow data is now provided. According to Smirnov et al. (2001), a three-dimensional transient flow field, $u_i(x_j, t)$, can be obtained from,

$$u_i(x_j, t) = \sqrt{\frac{2}{n=N}} \sum_{n=1}^N \left[p_i^n \cos(\hat{k}_j^n \hat{x}_j + \omega_n \hat{t}) + q_i^n \sin(\hat{k}_j^n \hat{x}_j + \omega_n \hat{t}) \right], \quad (6)$$

where the following non-dimensional quantities have been introduced, $\hat{x}_j = x_j/l_t$; $\hat{t} = t/\tau_t$; $c = l_t/\tau_t$; $\hat{k}_j^n \hat{x}_j = k_j^n \hat{x}_j c/c_{(j)}$, where, $p_i^n = \varepsilon_{ijm} \zeta_i^n k_m^n$; $q_i^n = \varepsilon_{ijm} \xi_i^n k_m^n$, with, $\zeta_i^n, \xi_i^n, \omega_n \in N(0, 1)$, $k_i^n \in N(0, 1/2)$. Note that $N(M, \sigma)$ denotes a normal distribution with mean M and standard deviation σ . Repeated sub-indexes imply summation, following Einstein's rule, while parentheses around indexes preclude summation. In these non-dimensional expressions, l_t and τ_t denote the characteristic length and time scales of turbulence, respectively, ε_{ijk} is the permutation tensor used in the vector product operation, c_i denotes the fluctuating velocity components written in a new system of coordinates, which is obtained after the application of the transformation tensor a_{ij} . The numbers k_j^n , ω^n represent a sample of n wave-number vectors and frequencies of a modeled turbulence spectrum $E(k) = 16(2/\pi)^{1/2} k^4 \exp(-2k^2)$. The final flow field u_i is obtained after scaling and orthogonal transformation operations: $u_i = a_{ij} w_j$, where $w_j = c_{(j)} v_{(j)}$. It is important to note that the tensor a_{ij} is such that $a_{mi} a_{nj} R_{ij} = \delta_{mn} c_{(n)}^2$, and $a_{ik} a_{kj} = \delta_{ij}$, where R_{ij} is a prescribed velocity correlation tensor, e.g., the Reynolds stress tensor. It is also worth noting that this procedure requires specifying the characteristic integral length and time scales of turbulence, and the correlation tensor R_{ij} of the flow. These quantities can be obtained from experimental data, but some of them may also be approximated from preliminary RANS simulations. A

323 similar framework has been retained by Batten et al. (2004) to address the
 324 couplings between RANS and LES closures. This strategy has been applied
 325 with some success to the computation of a turbulent channel flow by Keat-
 326 ing et al. (2004). The corresponding numerical simulation has been conducted
 327 with $N = 200$ Fourier modes, see Eq.(6), and a relatively long transition region
 328 has been required to regenerate fully-developped turbulence downstream of the
 329 inlet. Finally, assuming a modified von Kármán spectrum, a similar methodol-
 330 ogy has been also proposed by Davidson and Billson (2004) to generate *forcing*
 331 *conditions* at the matching boundary between the LES and URANS regions of
 332 hybrid numerical simulations. There is still today a fast-growing literature on
 333 the interfacing between RANS and LES methods and the present manuscript
 334 does not allow us to review it in further detail. The interested reader may find
 335 a rather complete view of this topic in the survey chapter of the book of Sagaut
 336 et al. (2006) and references therein.

337 2.2.4. *Synthetic eddy method - SEM*

338 The synthetic eddy method (SEM), proposed by Jarrin et al. (2009), is based
 339 on the decomposition of the turbulent flow field into stochastic coherent struc-
 340 tures. The corresponding eddy-structures are generated at the computational
 341 domain inlet plane and defined thanks to a shape-function $f_\sigma(x)$, which is in-
 342 tended to encode turbulence spatial and temporal characteristics.

343 The SEM can be introduced using a one-dimensional scheme, in which the
 344 velocity component is generated within the range $[a, b]$. The shape-function of
 345 each turbulent spot features a compact support in $[-\sigma, \sigma]$ and it satisfies the
 346 normalization condition.

$$\frac{1}{\Delta} \int_{-\Delta/2}^{\Delta/2} f_\sigma^2(x) dx = 1, \quad (7)$$

347 where $\Delta = b - a + 2\sigma$. Each turbulent spot has a position $x^{(n)}$, a length scale σ
 348 and is assigned a signal $\epsilon^{(n)}$. In other words, the contribution $u^{(n)}(x)$ of a tur-
 349 bulent spot n to the velocity field, is defined as $u^{(n)}(x) = \epsilon^{(n)} f_\sigma(x - x^{(n)})$, with
 350 a location $x^{(n)}$ randomly chosen within the range $[a - \sigma, b + \sigma]$ and where $\epsilon^{(n)}$

351 denotes a random step of value -1 or $+1$. The synthetic eddies are generated
 352 in an interval larger than $[a, b]$. This larger interval guarantees that the inlet
 353 points are surrounded by eddies. Finally, the resulting velocity field $u(x)$ at any
 354 location will be the sum of the contributions of all synthetic eddies located in
 355 the domain, $u(x) = \sum_{n=1}^{n=N} \epsilon^{(n)} f_{\sigma}(x - x^{(n)})/\sqrt{N}$, where N denotes the total num-
 356 ber of synthetic eddies. In three-dimensional situations, the generated eddies
 357 correspond to three-dimensional structures, which feature a compact support
 358 $[-\sigma_{x_1}, \sigma_{x_1}] \times [-\sigma_{x_2}, \sigma_{x_2}] \times [-\sigma_{x_3}, \sigma_{x_3}]$, and satisfy a normalization condition
 359 similar to Eq. (7). Considering an inlet plane of dimensions $[0, L_{x_2}] \times [0, L_{x_3}]$,
 360 located at $x_1 = 0$, the position $(x_1^{(n)}, x_2^{(n)}, x_3^{(n)})$ of the synthetic eddy n is ran-
 361 domly chosen within $[-\sigma_{x_1}, \sigma_{x_1}] \times [-\sigma_{x_2}, L_{x_2} + \sigma_{x_2}] \times [-\sigma_{x_3}, L_{x_3} + \sigma_{x_3}]$. The
 362 eddies are convected through the inlet plane at a velocity U_0 obtained from
 363 Taylor's hypothesis $x_1^{(n)}(t + \Delta t) = x_1^{(n)}(t) + U_0 \Delta t$. Once $x_1^{(n)}(t + \Delta t) > \sigma_{x_1}$,
 364 the eddy is re-generated at $x_1 = -\sigma_{x_1}$, and can be convected again. Finally
 365 the fluctuating velocity field is given by $u'_j(\mathbf{x}, t) = \sum_{n=1}^{n=N} \epsilon_j^{(n)} f_j(\mathbf{x} - \mathbf{x}^{(n)}(t))/\sqrt{N}$,
 366 where $\epsilon_j^{(n)}$ corresponds to the signal, i.e. -1 or $+1$, of the eddy n in direction j .
 367 The final velocity field u_i is then obtained from the above synthetic fluctuating
 368 velocity field u'_j , the velocity mean profile $\tilde{u}_i$, and the Cholesky's decomposition
 369 a_{ij} of the Reynolds stress tensor: $u_i = \tilde{u}_i + a_{ij}u'_j$, with a_{ij} defined by Eq. (2).

370 **3. Mathematical and computational modelling**

371 The mathematical and computational framework retained to proceed with
 372 the numerical simulation is now briefly presented. The interested reader may
 373 find a detailed presentation elsewhere (Vedovoto et al., 2011). A hybrid ap-
 374 proach in which the LES methodology is coupled with the transport of the scalar
 375 probability density function (PDF) is retained to describe the reactive cases.
 376 The method involves the numerical solution of partial differential equations
 377 (LES solver) together with stochastic differential equations (PDF solver). From
 378 the LES approach the Eulerian filtered variables are evaluated while stochastic
 379 differential equations (SDE) are solved using Lagrangian notional particles to

380 simulate the modelled transport equation of the scalar PDF (Pope, 1985; Colucci
 381 et al., 1998). The latter yields the one-point, one-time statistics of subgrid-scale
 382 scalar fluctuations and thus provides the LES solver with the corresponding
 383 filtered chemical reaction rate.

384 3.1. Mathematical model

385 The present section is organized as follows: the filtered set of balance equa-
 386 tions that describes the flows under consideration is first presented. The main
 387 characteristics of the transported PDF method are then briefly introduced to-
 388 gether with the equivalent system of stochastic differential equations as well as
 389 the coupling between the Eulerian and Lagrangian approaches (LES-PDF).

390 3.1.1. Set of filtered equations

391 The following simplifying assumptions are used: (a) fluid is considered as
 392 Newtonian, (b) body forces, heat transport by radiation, Soret and Dufour ef-
 393 fects are not addressed, (c) the model is developed for low Mach number flows,
 394 (d) we consider unity Lewis number values and equal molecular diffusion coeffi-
 395 cients for all species, (e) heat losses are neglected. The mathematical model con-
 396 siders multi-species variable-density reactive flows, in which the primary trans-
 397 ported variables are the density ρ , the three velocity components u_i , the specific
 398 enthalpy h and the mass fractions Y_k of the K chemical species ($k = 1, \dots, K$),
 399 the balance equations are:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0, \quad (8)$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{u}_i}{\partial x_j} = \frac{\partial \bar{T}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}^{SGS}}{\partial x_j}, \quad (9)$$

$$\frac{\partial \bar{\rho} \tilde{\phi}_\alpha}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}_\alpha}{\partial x_j} = \frac{\partial \bar{Q}_{\alpha,j}}{\partial x_j} - \frac{\partial Q_{\alpha,j}^{SGS}}{\partial x_j} + \bar{S}_\alpha, \quad (10)$$

402 where the variable ϕ_α denotes the mass fraction of a chemical species or the
 403 enthalpy of the mixture, $(x_i, i = 1, 2, 3)$ are the spatial coordinate, and t is the
 404 time. $T_{ij} = \tau_{ij} - p \delta_{ij}$ is the tensor of mechanical constraints including both a
 405 deviatoric (shear stresses τ_{ij}) and a spheric (pressure $p \delta_{ij}$) contribution, while

406 $Q_{\alpha,j}$ denotes the component of the molecular diffusion flux of the scalar α in
 407 the direction j . In the above expression, $\tau_{ij}^{SGS} = (\overline{\rho u_i u_j} - \bar{\rho} \tilde{u}_i \tilde{u}_j)$ is the subgrid
 408 scale (SGS) stress tensor and $Q_{\alpha,j}^{SGS} = (\overline{\rho u_i \phi_\alpha} - \bar{\rho} \tilde{u}_i \tilde{\phi}_\alpha)$ represents the SGS
 409 scalar flux components, respectively. Finally, the last term in the RHS of Eq.
 410 (10), i.e. $\bar{S}_\alpha$, denotes the filtered reaction rate. The above system is completed
 411 by an equation of state: $P = P_0(t) + p(\mathbf{x}, t)$, with $P_0(t)$ the thermodynamic
 412 pressure.

413 The unresolved momentum fluxes are expressed according to the Boussi-
 414 nesq assumption, $\tau_{ij}^{SGS} - \delta_{ij} \tau_{kk}^{SGS} / 3 = 2\mu_{SGS} (\tilde{S}_{ij} - \delta_{ij} \tilde{S}_{kk} / 3)$, where μ_{SGS} is the
 415 subgrid scale viscosity, and $\tilde{S}_{ij} = (\partial \tilde{u}_i / \partial x_j + \partial \tilde{u}_j / \partial x_i) / 2$ is the strain rate ten-
 416 sor of the resolved field (Ferziger and Peric, 1996; Fureby, 2008). In most of
 417 the numerical simulation results presented below, the eddy viscosity μ_{SGS} is
 418 obtained from the Smagorinsky closure, i.e., assuming that the small scales
 419 are in equilibrium, so that energy production and dissipation are in balance,
 420 which yields, $\mu_{SGS} = \bar{\rho} (C_s \Delta)^2 |\tilde{S}| = \bar{\rho} (C_s \Delta)^2 (2\tilde{S}_{ij} \tilde{S}_{ij})^{1/2}$, where C_s denotes
 421 the Smagorinsky constant. It is known that this closure can be excessively
 422 dissipative, especially near the walls, which is corrected herein by using a van
 423 Driest damping function (Ferziger and Peric, 1996). Finally, the SGS scalar
 424 flux is represented with a gradient law, $Q_{\alpha,j} = -\bar{\rho} \Gamma_{SGS} \partial \tilde{\phi}_\alpha / \partial x_j$, where $\tilde{\phi}_\alpha$ is the
 425 resolved scalar field and Γ_{SGS} denotes the subgrid diffusion coefficient evaluated
 426 from $\Gamma_{SGS} = \bar{\rho} (C_s \Delta)^2 |\tilde{S}| / Sc_{SGS}$ with Sc_{SGS} a subgrid scale turbulent Schmidt
 427 number.

428 The accurate determination of the filtered chemical reaction rate $\bar{S}_\alpha$ remains
 429 one of the most important challenges when applying LES to turbulent reactive
 430 flows. We retain herein a formulation that accounts for the subgrid scale fluc-
 431 tuations of the chemical composition through a modelled transport equation
 432 for the subgrid scale PDF, which provides an effective resolution to the closure
 433 problems that arise from averaging or filtering the highly nonlinear chemical
 434 source terms (Haworth, 2010). Since one-point one-time PDF models are used,
 435 the terms that involve two points information, i.e., some property gradients, are
 436 not explicitly resolved, hence important effects, such as molecular diffusion and

viscous effects, and associated dissipation phenomena require to be modeled.

The modelled transport equation for the scalar PDF is written as:

$$\begin{aligned}
\frac{\partial}{\partial t} \rho(\Psi) P_{\Phi}(\Psi; \mathbf{x}, t) &+ \frac{\partial}{\partial x_j} \rho(\Psi) \tilde{u}_j P_{\Phi}(\Psi; \mathbf{x}, t) \\
&= \frac{\partial}{\partial x_j} \left[\rho(\Psi) (\Gamma + \Gamma_{SGS}) \frac{\partial P_{\Phi}(\Psi; \mathbf{x}, t)}{\partial x_j} \right] \\
&+ \frac{\partial}{\partial \psi_{\alpha}} [\rho(\Psi) \Omega_m (\psi_{\alpha} - \langle \phi_{\alpha} \rangle) P_{\Phi}(\Psi; \mathbf{x}, t)] \\
&- \frac{\partial}{\partial \psi_{\alpha}} [S_{\alpha}(\Psi) P_{\Phi}(\Psi; \mathbf{x}, t)], \tag{11}
\end{aligned}$$

where the chemical reaction term appears in closed form, thus circumventing the difficulties associated with the physical modelling of its filtered contribution. The derivation of such a transport equation may be found elsewhere (Haworth, 2010). The retained hypotheses are: (i) the conditional filtered velocity has been decomposed into filtered and subgrid contributions, with the latter closed by a turbulent diffusivity approximation, (ii) the conditional mixing term is closed by the IEM mixing model Villermaux and Devillon (1972) also often referred to as the linear mean-square estimation (LMSE) model (Dopazo and O'Brien, 1974). In the above equation, $\Omega_m = C_{\omega} (\Gamma + \Gamma_{SGS}) / \Delta^2$ denotes the turbulent mixing frequency, with $C_{\omega} = 2.0$ the mechanical to scalar time scale ratio (Raman, 2004).

3.1.2. Lagrangian Monte Carlo approach

The Lagrangian Monte Carlo approach offers the most classical framework to deal with the above PDF transport equation (Pope, 1985; Fox, 2003). In this approach, the joint scalar PDF is represented by an ensemble of notional particles (Fox, 2003), which evolve according to equivalent stochastic differential equations (SDE). A general framework to construct SDEs that are equivalent to the PDF transport equation is provided by Gardiner (2009).

In the present context, the SDEs that describe the trajectory of the particles in the physical space, $\mathbf{x}$, and in the sample space of the scalar field, Ψ , can be written as:

$$d\mathbf{x} = \left[\tilde{\mathbf{u}}(\mathbf{x}, t) + \frac{\partial \Gamma_{SGS}}{\partial x_i} \right] dt + \sqrt{2\Gamma_{SGS}} d\mathbf{W}(t), \tag{12}$$

$$d\Psi = [-\Omega_m (\Psi - \langle \Phi \rangle) + S(\Psi)/\rho(\Psi)] dt \quad (13)$$

where $\mathbf{W}(t)$ denotes the Wiener process, associated with a Gaussian random variable featuring zero mean value and a variance dt (Fox, 2003). The evolution of each notional particle occurs according to statistically independent increments $d\mathbf{W}(t)$, with a subgrid scale diffusion coefficient evaluated from the LES solver. The possible restrictions associated with the use of such an approach have been extensively discussed by Haworth (2010).

3.2. Numerical model

This section reports the essential features of the numerical solver *FLUIDS_3D* that has been used to conduct the numerical simulations reported hereafter. The reader may refer to Vedovoto et al. (2011) for further insights on the Eulerian solver.

3.2.1. Navier-Stokes equations (NSE) solver

The numerical method is based on a three-dimensional, conservative, staggered, finite-volume discretization (Ferziger and Peric, 1996). In the present work, a fully implicit scheme is retained, which requires the numerical resolution of a large algebraic system; the MSIP - Modified Strongly Implicit Procedure (Schneider and Zedan, 1981) is retained to this purpose.

In the low Mach number flows under consideration, the density is solely determined by the temperature and thermodynamic pressure fields P_0 . The energy equation plays the role of an additional constraint on the velocity field, which is enforced by the dynamic pressure. This constraint acts onto the velocity field divergence, and it is related to the total derivative of the density, see Vedovoto et al. (2011). Once the pressure correction is evaluated, the velocity field can be updated.

The present numerical simulations are conducted with a central difference scheme (CDS) to represent the spatial derivatives. Time integration is performed using the backward difference scheme (BDF) with a CFL number value set to 0.5. Further information about the available discretization procedures, as

well as the verification of the numerical code developed can be found in Vedovoto et al. (2011).

3.2.2. Stochastic differential equations (SDE) solver

The Lagrangian stochastic particles move through the physical space independently of each other. They are assigned spatial coordinates and represent mass. Due to the stochastic nature of motion, the number of particles present in a given elementary volume changes in time. In order to prevent particle accumulations in computational cells, and to keep small computational cells from running empty, particles are ascribed a relative weight (Zhang and Haworth, 2004). Following Pope (1985), the SDEs are discretized resorting to a fractional step method. For instance, Eq.(12) is re-written as $dx_i = A(X(t))dt + B(X(t))dW_i(t)$. The stochastic nature of this equation is associated with the Wiener process W_i . The increments of the Wiener process, $dW_i(t + \Delta t) = W_i(t + \Delta t) - W_i(t)$, with $i = 1, \dots, N_w$, where N_w is the number of independent processes, drive the evolution of the particle in physical space. According to the model equation (11), the drift, $A(X(t))$, and diffusion coefficients, $B(X(t))$, are defined as, $A(X(t)) \equiv [\tilde{u}_i + \partial(\Gamma + \Gamma_{SGS})/\partial x_i]$, and, $B(X(t)) \equiv \sqrt{2(\Gamma + \Gamma_{SGS})}$. The most widespread discretization procedure retained for such equations is the Euler-Maruyama method (Gardiner, 2009). However, such a method, in its explicit formulation, requires very small time steps due to stability issues. The present numerical simulations rely on the Milstein scheme (Kloeden and Platen, 2000) which has a strong and weak order of convergence equal to unity. Applying the Milstein scheme to Eq.(12) gives rise to the following discretized form $dx_i = A(X(t))\Delta t + B(X(t))\Delta W_i + 0.5 B'(X(t))B(X(t))((\Delta W_i)^2 - \Delta t)$, where $B'(X(t))$ is the first derivative of $B(X(t))$ with respect to time.

3.3. Implementation of the synthetic turbulence generators. Discussion.

Four distinct turbulence generators have been implemented in the Navier-Stokes solver *FLUIDS_3D*. Among them, the simplest and still most widely-

517 used WN model simply consists in superimposing a white noise onto the mean
 518 velocity profile. However, its low computational cost and ease of implementation
 519 unfortunately cannot compensate for its poor representativeness, mainly due to
 520 its lack of energy at small wavenumbers, which may postpone any transition to
 521 turbulence.

522 As far as more realistic synthetized turbulence procedures are concerned,
 523 we will now discuss and compare the ease of both implementation and use of
 524 the DF, RFG and SEM procedures. The first method, i.e., the DF model,
 525 has been implemented from scratch in the *FLUIDS_3D* solver. It obviously
 526 demands a little bit more programming skills than those required to encode
 527 the WN model. However, its practical use remains quite simple provided that
 528 a detailed preliminary analysis of the sensitivity to the filter support size is
 529 conducted for the geometry of interest. In comparison with the WN model, it
 530 should be noted that the DF, RFG and SEM models all require to be fed with
 531 the Reynolds stress tensor components. In terms of computational performance,
 532 the DF method suffers from an important CPU cost, which is the highest among
 533 the different method that have been considered. This CPU cost increases at the
 534 power N^3 with N the size of the filter support.

535 Since it has been performed on the basis of an original set of RFG routines
 536 written in C programming language, the practical implementation of the RFG
 537 method was rather simple. Special care must be taken to avoid any misuse of
 538 data types as soon as C and fortran exchanges are required. The method is of
 539 very simple use and, if we except the WN model, it was found the most efficient
 540 among those implemented. It is worth recalling that all simulations carried out
 541 in this work make use of parallel processing. This is a quite important point
 542 since the CPU costs of the synthetic turbulence procedures used at the inlet
 543 of the computational domain may indeed lead to important unbalanced loads.
 544 This is a serious issue with respect to the use of the DF method. It has been
 545 noticed that, with the DF method, the computational sub-domains lying at the
 546 inlet require about 10 per cent more random access memory (RAM) than the
 547 others.

Finally, the last method considered is the SEM method. It has also been implemented from scratch in the *FLUIDS_3D* solver. In terms of complexity of implementation we must recognize that, given the amount of information available in the literature, this task is very affordable. The computational cost of the SEM is found comparable to the one of the RFG method. As shown and discussed later on, the capacity of generating an energy spectrum that mimics some desirable characteristics, such as an inertial zone featuring a $-5/3$ power-law decay rate as well as the capability of the SEM to recover a prescribed anisotropic tensor makes the method very appealing. In addition to this, the obtained results display only a rather small dependence on the number of eddies generated, which contributes to maintain the CPU costs reasonable.

4. Application to homogeneous isotropic turbulence

In the present brief section, we proceed with a preliminary inspection of the inflow generator capabilities for the case of a spatially decaying isotropic turbulence. The conditions studied herein are very similar to the ones previously considered by Jarrin et al. (2009) and the reader may refer to this archival publication for further details. The mean flow is oriented towards the positive x_1 -direction. The computational domain is a three-dimensional box with characteristic dimensions $(20 \times 6 \times 6)$, discretized with a finite volume mesh featuring $200 \times 60 \times 60$ cells in the x_1 , x_2 and x_3 -directions, respectively. The mesh is homogeneous in all three directions. Periodic boundary conditions are imposed along the x_2 and x_3 -directions. An unsteady advective (also often denoted convective) boundary condition is applied on the outflow plane ($x_1 = 20$). This unsteady boundary condition determines a velocity field that ensures an outflow mass flux equal to the incoming mass flux. The implemented formulation is the one proposed by Orlanski (1976). The mean streamwise velocity is set to $U_0 = 20 \text{ m/s}$, and the molecular viscosity is $\nu = 3.5 \times 10^{-4} \text{ m}^2/\text{s}$. The mean turbulent kinetic energy at the inlet is $k_0 = 3/2 \text{ m}^2/\text{s}^2$ and finally, for the simulation results presented below, the integral length scale is set to $L = 0.4 \text{ m}$.

577 It seems worth emphasizing that these values are exactly the same as those
 578 previously retained by Jarrin et al. (2009). Statistics are averaged over two
 579 flow-through domain times and over homogeneous periodic directions.

580 The set of results gathered in Fig. 1 displays the influence of the inflow tur-
 581 bulence generators. The energy spectra are extracted at five distinct locations
 582 in the computational domain. The five probes are located at $x_1 = 0.05$, i.e., in
 583 the first control volume immediately downstream of the inlet plane, and further
 584 downstream at positions $x_1 = 1$, $x_1 = 5$, $x_1 = 9$, and $x_1 = 19$. The x_2 and
 585 x_3 -coordinates of the probes are held constant and equal to 3, i.e., positioned
 586 in the middle of the computational domain cross-section.

Figure 1: One-dimensional longitudinal energy spectra (u_1 -component of velocity). The sub-figures (a), (b), (c) and (d) correspond to the results of simulations obtained at $x_1 = 1$, $x_1 = 5$, $x_1 = 9$, and $x_1 = 19$ respectively. WN (blue curve); DF (green curve), RFG (black curve) and SEM (red curve).

587 To perform the comparative analysis, the white noise synthetic turbulence
 588 generator is considered with a fluctuation level of twenty per cent imposed on the

streamwise component of the velocity field, while 10 per cent fluctuations are set for the components in the x_2 and x_3 -directions. For the simulations conducted with the DF method, the size of the filter support is set to 10 while 1,000 Fourier modes are retained for the simulations based on the RFG method. For the simulation carried-out with the SEM, 10000 eddies are used. Time integration is performed using the Backward Difference Scheme with a CFL number value set to 0.5. The advective terms of the transport equations are discretized by using the CDS approach. Finally, since the numerical code developed has the capability of performing distributed computing, the computational domain is divided into 16 sub-domains.

From Fig. 1, it is clear that, for the probe positioned at $x_1 = 19$, the effects associated with the choice of one given inflow turbulence generator are minimized. At this position, the energy spectrum is indeed developed, i.e, the turbulent flowfield got enough time *to forget* the influence of the highest frequencies that were introduced through the synthetic inlet turbulence signals¹. This offers quite a remarkable contrast with the spectra observed at the inlet ($x_1 = 0.05$) where strong differences may be observed and the effects of the inflow generator are very revealing. In fact, with the exception of the RFG model, it is worth noting that the different methods fail to display a satisfactory spectral behavior just downstream of the inlet. To conclude with this preliminary investigation, the values of the velocity derivative skewness are inspected, see Fig. 2. This quantity is related to vortex stretching and energy transfer. The value obtained at $x_1 = 19$ for the white noise is very small: $S = -0.030$. With the WN procedure all the energy is dissipated after a few cells downstream the inlet. The inflow data indeed does not exhibit any spatial and/or temporal correlation: two neighbouring points are uncorrelated, which leads to high velocity gradients and a quasi-instantaneous dissipation of turbulent kinetic energy at the inlet plane. This behavior simply confirms that the small computational cost of the WN model cannot compensate for its inability to reproduce even

¹The obtained level of fluctuations still appears to be quite altered with the WN model.

the simplest statistics of the turbulent flow field. In contrast, we measured $S = -0.215$ at the same location ($x_1 = 19$) for the DF model, $S = -0.268$ for the RFG model and $S = 0.161$ for the SEM. Such values are comparable to those previously documented by Jarrin et al. (2009).

Figure 2: Downstream evolution of the (a) turbulent kinetic energy spatial decay rate (top), and (b) the velocity derivative skewness (bottom) plotted versus the longitudinal coordinate $x_1(m)$; (—) WN, (---) DF, (···) RFG, and (—) SEM.

5. *A priori* analysis of the turbulent inflow data generators

The influence of turbulence inlet generators is now investigated in condi-

tions relevant to practical applications and we will compare resulting statistics
 in a simplified configuration so as to assess the efficiency of the models. Before
 examining the effect of the inflow generation technique on flowfields computed
 in a representative geometry, we present below comparative analyses of the
 implemented turbulent inflow data generators. The experimental stress tensor
 profile and mean velocity characteristics retained for testing the turbulent inflow
 generation techniques are based on the experimental studies conducted in the
 geometry of Moreau, see Magre et al. (1988). The corresponding experimental
 setup offers a reference test case (Bilger et al., 2005). For instance Andrade
 et al. (2011) performed the LES of the corresponding flowfield by resorting to
 a classical white noise generator and the present investigation may therefore be
 helpful to get a better understanding of the residual differences they observed
 between experiments and computational results. The experimental test section
 permits the development of a high speed turbulent mixing layer, where a pre-
 mixed methane-air flow can be ignited and stabilized by a parallel stream of
 combustion products. Profiles of mean velocity, turbulence intensity and ve-
 locity fluctuations have been characterized for both reactive and non-reactive
 flows. Experimental data make available the R_{11} component of the Reynolds
 stress tensor only. Andrade et al. (2011), when simulating this configuration,
 assumed that the R_{22} and R_{33} components are approximately half of the R_{11}
 component. The components $R_{12} = R_{21}$ and $R_{32} = R_{23}$ are taken as zero.
 These assumptions are retained here. No information is given about the cross
 component R_{13} , but since it plays a crucial role in the shear layer spreading
 rate, we must satisfactorily approximate such a quantity. Brucker and Sarkar
 (2007) provide a relation in which the non-dimensional width of the shear layer,
 $\xi = h/\delta_m$, with h varying between $[-\delta_m < h < \delta_m]$, is correlated to the non-
 dimensional quantity $R_{13}/\Delta\bar{u}_1^2$ in self-similar mixing layers. Once defined the
 velocity difference between two streams, $\Delta\bar{u}_1^2$, and the width of the mixing layer
 $\delta_m = 5$ mm, the component $R_{13} = R_{31}$ can be evaluated from Brucker and
 Sarkar (2007) data.

The combustion chamber is a channel with dimensions $800 \times 100 \times 100$ mm³

655 in the directions x_1 , x_2 and x_3 respectively. The inlet is divided into two ducts
 656 separated by a splitter plate. The fresh gases are injected at 65 m/s in the main
 657 (upper) duct while hot gases, featuring a mean velocity of 130 m/s, are injected
 658 in an auxiliary duct, see Fig. 3. For the present test, which aims at evaluating
 659 the variables of interest at the inlet plane only, the two-dimensional grid is
 660 divided into 50 points in the x_2 -direction and 50 points in the x_3 -direction. The
 661 mean velocity profile used at the inlet is represented by a combination of two
 662 developed flows at different exit velocities. The analytical function adopted for
 663 generating the corresponding mean velocity profile is,

$$\tilde{u}_1(x_3) = C_{in} \left[1 - \left(\frac{x_3 - (a/2 + h)}{a/2} \right)^{\gamma_{in}} \right], \quad (14)$$

664 where C_{in} is the mean value of the velocity in the duct, a is the position of the
 665 bottom part of the duct in the x_3 -direction, h is the height of the duct, and γ_{in}
 666 is a constant that sets the thickness of the shear layer. The values of the above
 667 parameters are summarized in Table (1).

Figure 3: Computational domain retained to perform the numerical simulations (left), and mean velocity profile imposed at its inlet (right); $x_3^* = x_3/\delta_m$ denotes the non-dimensional coordinate with δ_m the initial width of the mixing layer

668 As stressed above, it is important to verify if the procedures implemented
 669 for generating the turbulent inflow data reproduce a random signal in which
 670 the energy spectrum distribution corresponds to more energetic scales in the
 671 smallest wave numbers, and to less energetic scales in the highest wave numbers.

Moreover, the capability to generate a prescribed Reynolds stress tensor is also of paramount importance.

Table 1: Values of the parameters associated with the imposed mean velocity profile.

Duct	C_{in} [m/s]	h [m]	a [m]	γ_{in}
Main duct	65	0.02	0.08	6.0
Auxiliary duct	130	0.00	0.02	8.0

The DF and RFG methods feature some factors that directly impact both the accuracy in reproducing the characteristics of the flows of interest and the associated computational cost. Concerning the former, the main factor is the filter support size, and for the latter, i.e., the RFG method, the number of Fourier modes in Eq. (6). For the SEM, the number of eddies may be expected to be the critical parameter. Given a set of initial conditions, e.g., mean velocity distribution, size and number of control volumes of the computational domain at the inlet, Reynolds stress tensor, characteristic length and time scales of a flow, the turbulent inflow generators are used to recover the statistics of the flow properties of interest by a classical averaging procedure applied on 5000 samples. In the present work, to reduce the computational cost, an isotropic signal is generated, and then Eqs. (1) and (2) are applied to the resulting signal in order to obtain the desired level of anisotropy.

5.1. WN model

The first and simplest method is the superimposition of a white noise on the mean velocity profile given by Eq. (14). In this case, a random signal with zero mean and unity variance is adjusted to yield fluctuations representing 20 per cent of the mean velocity in the x_1 -direction of the flow, i.e., the u_1 -component of velocity. In the x_2 and x_3 -directions, the fluctuations levels are set to 10 per cent of the mean velocity. Figure 4 displays a one-point temporal spectrum obtained from the energy of velocity fluctuations, i.e., $k(t) = 1/2 (u_1'^2(t) + u_2'^2(t) + u_3'^2(t))$, which has been sampled from a probe placed in the middle of the inlet plane. Note that the corresponding samples

697 were selected in such a manner that they are equally-spaced in time and the
698 frequency of data sampling has been optimized to restrict any possible loss of
699 information. As illustrated in this figure, the fact that the energy is spread over
700 the whole energy spectrum, whatever the fluctuation frequency, contradicts the
701 classical Kolmogorov description of turbulent flows.

Figure 4: Energy spectrum associated with a WN generator.

702 As expected, the lack of spatial or temporal correlations, added to the
703 isotropic nature of this process, leads to rather poor results when the com-
704 ponents of the computational stress tensor, as evaluated from the averaging
705 process of the inlet signal, are compared with experimental results, see Fig. 5.
706 Therefore, it can be foreseen that the use of the WN technique will lead to
707 poor results when applied to the full numerical simulation of the corresponding
708 experimental benchmark.

709 5.2. *DF model*

710 With the DF method, we may expect a certain degree of dependency of the
711 results on the filter support size. Since the filter size is directly connected to
712 the number of grid points at the inlet, the computational cost associated with
713 the number of points in the support, therefore, is an important issue. As it can

714 be seen in Fig. 6, as the support size is increased, the energy spectrum becomes
715 more representative of the one associated with a fully developed turbulent flow.

Figure 5: Stress tensor components evaluated from the white noise superimposition on the mean velocity profile; symbols $\bullet$: experimental data from Moreau and Boutier (1977); line: WN results.

716 Within the DF framework, the filter support size and the integral length
717 scale are interrelated through the expression of the filter coefficients b_j , and

as expected, with $N = 1$, the correlation is truncated to zero and the energy spectrum thus exhibits little difference from a white noise spectrum. The differences become more pronounced for N equal to 5, 10 and 20. For a given level of resolution, the influence of an increase in the filter support size is indeed similar to an increase of the turbulent length scale.

Figure 6: Influence of the support size N on the energy spectrum obtained with the DF method: (a) $N=1$, (b) $N=5$, (c) $N=10$, (d) $N=20$.

Concerning the computational cost of the DF method, in the tests carried out to evaluate the sensivity to the number of points N in the filter support, we obtain the following results: for $N = 1$, the code spent approximately one minute (using a CPU Intel (R) Xeon (TM) 3.00GHz with 4 gigabytes of RAM memory) to perform the 5000 iterations required to evaluate the statistics, whereas, for $N = 20$, for the same number of iterations, using the same computer, approximately 14 hours and 30 minutes were necessary.

Such a disparity can be easily understood by using a very simple example. For $N = 5$, a cubic box of dimensions $5 \times 5 \times 5$ is created for each point at the inlet. Since, in the present configuration, the inlet is composed of a grid of 50×50 points in x_2 and x_3 -directions, respectively, the total number of points

734 where the filtering process is performed is $50 \cdot 50 \cdot (5 \cdot 5 \cdot 5)$, or, 312,500 points.
735 For $N = 20$ this number becomes 2×10^7 points, which is 64 times larger.

Figure 7: Stress tensor components evaluated from the DF method ; • experimental data from Moreau et al (1977); Red curve: $N=1$; Blue curve: $N=5$; Magenta curve: $N=10$ and Black curve: $N=20$

736 Concerning the capability of the DF method to reproduce anisotropic stress
737 tensors, it can be seen in Fig. 7 that the support size influence is clearly less ob-

738 vious than the effects previously evidenced in the energy spectrum. It is indeed
 739 observed that, for filter supports larger than 10 points, no further improvement
 740 is obtained. From this preliminary analysis it is therefore suggested to retain a
 741 support size of 10 points for the subsequent numerical simulations.

Figure 8: Stress tensor components evaluated from the RFG method, influence of the number of Fourier modes: • experimental data from Moreau and Boutier (1977); Red curve: 50 Fourier modes; Blue curve: 500 Fourier modes; Magenta curve: 1000 Fourier modes and Black curve: 5000 Fourier modes

742 5.3. RFG model

743 For the tests presented in the this section, the RFG model is not found to be
 744 very sensitive to the number of Fourier modes retained, in terms of its ability
 745 to reproduce the prescribed stress tensor, as well as the shape of a turbulent
 746 spectrum, as can be seen in Figs. (8) and (9), respectively. Note that N stands
 747 for the number of Fourier modes retained in one single direction, and the same
 748 number of modes is considered in the three directions.

749 When a turbulent flow is analyzed in terms of Fourier modes, each mode can
 750 be understood as a particular turbulent scale. From Fig. 8, it is confirmed that,
 751 even a small number of Fourier modes provides a satisfactory reproduction of
 752 the prescribed stress tensor. Above 500 Fourier modes the differences observed
 753 between experimental data and computational results become completely in-
 754 significant.

Figure 9: Influence of the number of Fourier modes on the energy spectrum obtained with RFG method: (a) 50 Fourier modes, (b) 500 Fourier modes, (c) 1000 Fourier modes and (d) 5000 Fourier modes.

755 It can be noted in Fig. 9 that, as the number of Fourier modes is increased,
 756 the energy spectrum becomes more representative of that associated with high

757 Reynolds number turbulent flows. Moreover, it is observed in Fig. 9 that only
758 very slight differences persist when the number of Fourier modes exceeds 1,000.

Figure 10: Stress tensor components evaluated from the SEM model; • experimental data from Moreau et al (1977); Red curve: 100 eddies; Blue curve: 1000 eddies; Magenta curve: 10000 eddies and Black curve: 100000 eddies

759 To conclude, we found that obtaining turbulent inflow data featuring rep-
760 resentative energy spectra is computationally cheaper using the RFG model

761 than the DF model. For instance, the time spent to perform 5000 iterations,
 762 with 1,000 Fourier modes for obtaining computational statistics comparable to
 763 experimental data, is approximately five minutes. This is similar to the time
 764 consumed by the DF method, with a support $N = 5$, on the same Intel (R)
 765 Xeon (TM) 3.00GHz CPU with 4 gigabytes of RAM memory. Therefore, the
 766 numerical simulations reported in the next sections are performed with 1,000
 767 Fourier modes.

768 5.4. SEM model

769 As emphasized in section 2.2.4, the results obtained with this method are ex-
 770 pected to be sensitive to the turbulence characteristic length scale chosen. Such
 771 a quantity may be evaluated experimentally but, for the present application,
 772 this characteristic length scale is set to a constant value equal to $0.1 m$. This
 773 value was also the input parameter of the RFG method in the previous section.

Figure 11: Comparison of the effects of the number of eddies on the shape of the energy spectrum obtained with the SEM model. (a) 100 eddies, (b) 1000 eddies, (c) 10000 eddies, (d) 100000 eddies.

774 The SEM is subject to the same preliminary tests as those applied to the

DF and RFG methods. We study the capability of correctly reproducing the Reynolds stress tensor, and examine the shape of the resulting turbulent energy spectrum. It is possible to verify in Fig. 10 that a satisfactory representation of the Reynolds stress tensor can be obtained whatever the number of eddies initially prescribed, even with a total number of eddies varied between 100 (0.1k) and 100,000 (100k) eddies. Such an independence on the total number of eddies is also evidenced in Fig. 11. Indeed, the energy spectrum does not seem to be influenced by the number of modes, provided that it is larger than 100.

The computational cost, however, is found to vary linearly with the number of eddies. For 100k eddies, for instance, to perform 5000 iterations (using the same Intel (R) Xeon (TM) 3.00GHz CPU with 4 gigabytes of RAM memory), the time spent was about six minutes, while for 1k eddies, the code requires about 3 seconds only. In comparison with the calculations performed with the RFG and DF methods, the SEM appears thus to be considerably cheaper.

In the next sections we proceed with the analysis of the different turbulent inflow generators by conducting the LES of the experimental test case of Moreau and coworkers. In a first step of the analysis, the corresponding wall bounded turbulent mixing layer flows is investigated in non-reactive conditions and then attention is focused on the high-speed turbulent and reactive mixing layer.

6. Application to the numerical simulations of a wall bounded turbulent mixing layer flow

6.1. Sensitivity to the synthesized turbulence model

In order to assess the influence of the synthetic turbulence generators, three-dimensional numerical simulations of a high speed mixing layer are now performed. The obtained results are compared with the experimental data. The computational domain is a three-dimensional box with dimensions $(800 \times 100 \times 100)$ mm³, discretized with a finite volume mesh featuring $320 \times 100 \times 100$ cells in the x_1 -, x_2 - and x_3 -direction, respectively. Since the numerical code developed has the capability of performing distributed computing, the computational do-

main is divided into 40 sub-domains. No-slip boundary conditions are imposed in the x_2 and x_3 directions. An advective boundary condition is used at the outflow. The Smagorinsky model is used with $C_s = 0.18$, and the Van-Driest damping function is applied at the walls. The Reynolds number, based on the initial width of the mixing layer, $\delta_m = 5$ mm, the mean velocity difference between the two inlet streams $U_r = 97.5$ m/s and the value of the kinematic viscosity of air at 600 K is $Re = 3075$.

To perform the comparative analysis, the white noise synthetic turbulence generator is considered with fluctuation levels of 20 per cent and 10 per cent imposed on the streamwise and transverse velocity components respectively. For the simulations conducted with the DF method the size of the filter support is set to 10, whereas 1,000 Fourier modes are retained for the simulations based on the RFG method. For the simulation carried out using the SEM, 10k eddies are used. The mean velocity profile at the inlet is given by Eq. (14).

A probe is positioned just downstream of the computational domain inlet, in the first control volume along the x_1 -direction, and at $x_2^* = 10$ and $x_3^* = 4.6$. In Fig. 12 the normalized longitudinal filtered velocity component, i.e., $u^* = u/U_r$, is plotted against the normalized time, i.e. $t^* = tU_r/\delta_m$. In this figure the presence of high frequency structures appears to be more pronounced for the white noise, while it is less apparent for the velocity signal evaluated from the method of Klein et al. (2003). Moreover, one can notice in Fig. 12-(c) that there are almost no high frequencies in the velocity signal, which can be explained by the lack of energy that has been evidenced at the small scales in the decaying part of the energy spectrum, see Fig. 6. The same conclusion applies to the SEM.

Figure (13) displays the time-averaged filtered turbulent kinetic energy (TKE), evaluated from the trace of the Reynolds stress tensor, for the different methods retained to generate the inflow. The statistics are obtained by time averaging the filtered flow field over four flow-through (residence) times, resulting in ap-

835 approximately 15,000 realizations.

Figure 12: Temporal evolution of the u_1 component of velocity downstream of the flow inlet; (a) WN, (b) DF, (c) RFG, and (d) SEM.

836 It is noteworthy that the use of an improved method to generate the turbu-
837 lent inflow data drastically changes the flow field structure. For instance, in Fig.
838 13-(a) the TKE levels become significant after one half of the total length of the
839 computational domain in the x_1 -direction only, whereas for the DF and RFG
840 methods, the flow resembles that observed experimentally, see Fig. 13. Due
841 to the high level of turbulent intensity in the incoming ducts that inject fresh

842 and burnt gases streams into the combustion chamber, the turbulence at the
 843 inlet is fully developed. It is worth noting that in the comparisons henceforth
 844 shown concerning the Reynolds stress tensor components, the sub-grid contri-
 845 bution is also accounted for. The turbulent kinetic energy levels for the DF,
 846 RFG and SEM are also larger downstream of the inlet of the computational
 847 domain. Again, although a transition to turbulence is observed when the white
 848 noise generator is used, practically all velocity fluctuations entering the compu-
 849 tational domain are almost immediately dissipated close to the inlet boundary
 850 condition, and the first coherent structures are observed only after the first half
 851 length of the computational domain, along the x_1 -direction.

Figure 13: Fields of turbulent kinetic energy for the simulations carried out with the methods:
 (a) WN, (b) DF, (c) RFG and (d) SEM.

852 An instantaneous field of the normalized effective turbulent viscosity, i.e.
 853 $\mu_e^* = (1 + \mu_{SGS}/\mu)$, is reported in Fig. 14. It is clear from this figure that the

level of turbulence at the inflow is higher in sub-figures (b), (c), and (d). It can thus be concluded, that, since the Smagorinsky model is used, and since such model relies on the resolved strain rate to evaluate the sub-grid viscosity, the values of strain rate in the vicinity of the inlet of the computational domain is higher for the DF, RFG and SEM than when the white noise is considered.

Figure 14: Snapshot of the normalized effective turbulent viscosity μ_e at $t^* = 19500$, for the simulations carried out with the methods: (a) WN, (b) DF, (c) RFG and (d) SEM at $t = 1s$ ($t^* = 19500$).

Figure 15 displays an isovalue of Q , the second invariant of the velocity gradient tensor, which is colored by the velocity magnitude. It shows clearly that the WN is subject to a transition in the middle of the computational domain. In comparison with the RFG and SEM, it is also evident from this figure that there is a more significant turbulent activity just downstream of the inlet plane when the DF method is used.

Figure 15: Iso values of $Q = 2.5 \times 10^6$ colored by the filtered velocity magnitude for the methods (a) WN, (b) DF, (c) RFG and (d) SEM at $t = 1s$ ($t^* = 19500$).

Figure 16, which depicts the vorticity component along direction x_2 , also provides a valuable insight into the behavior of the Smagorinsky model. It is commonly agreed that the Smagorinsky model is highly dissipative. This is one of the reasons that also explains why the white noise generator signal imposed at the inlet may be rapidly destroyed. However, provided that a more elaborated method is retained to generate the inflow turbulence, Fig. 14 confirms that a signal featuring large scales introduced in the domain is not so quickly dissipated, even when the Smagorinsky model is used.

Figure 16: Component in x_2 -direction of the vorticity as obtained from the simulations carried out with the methods (a) WN, (b) DF, (c) RFG and (d) SEM at $t = 1s$ ($t^* = 19500$).

873 In order to assess more quantitatively the methods implemented, Fig. 17
874 displays comparisons of the averaged u_1 -component of the velocity with experi-
875 mental data at four distinct locations in the computational domain, for $x_2^* = 10$.
876 The results confirm that the different methods provide an acceptable representa-
877 tion of the mean velocity field when compared with experimental data. However
878 the need for an improved turbulent inflow generator becomes clear to recover
879 the levels of velocity fluctuations. Indeed, it can be seen in Fig. 18 that the
880 superimposition of white noise on the mean velocity is unable to recover the
881 experimental data in the first half of the computational domain along the x_1 -
882 direction - a conclusion that agrees with the previous work of Andrade et al.
883 (2011). In contrast, the results obtained with the DF, RFG and SEM display a
884 more satisfactory level of agreement with experimental data at the same loca-

tion. It is also worth noting the presence of two maximum values on the $\sqrt{R_{11}}$ profile, featuring a remarkable amplitude for the SEM. The first, positioned around $x_3^* = 5$, is associated with the shear layer growth, whereas the second develops in the vicinity of the wall.

Figure 17: Mean longitudinal velocity profiles obtained using the classical Smagorinsky model. (●): Experimental data (---) WN, (- -) DF, (..) RFG and (—) SEM.

Figure 18: $\sqrt{R_{11}}$ stress tensor component profiles obtained using the classical Smagorinsky model. (●): Experimental data (---) WN, (- -) DF, (..) RFG and (—) SEM.

889 From the computational cost point of view, it is clear that the better quality
 890 of the results obtained with the DF, RFG and SEM methods requires a non-
 891 negligible amount of CPU time. For the present test case, the simulations
 892 conducted with the DF and RFG methods correspond to approximately the
 893 same computational cost, i.e., about 40 per cent more than that associated with
 894 the white noise methodology, for the former, and 35 per cent for the latter.
 895 The cost associated with the numerical simulations conducted with the SEM
 896 is 55 per cent higher than that conducted with the white noise. The DF and
 897 RFG methods therefore, appear as very attractive. Nevertheless, there are
 898 two crucial differences between the DF and RFG methods. The first does not
 899 yield temporal correlations, only spatial correlations are guaranteed. Moreover,
 900 the RFG method generates a divergence-free velocity field at the inlet. This
 901 confirms that the RFG method is an excellent candidate to impose synthesized
 902 turbulence.

903 *6.2. Sensitivity to the SGS closure*

904 Whatever the intrinsic qualities and limitations of the synthetic turbulence
 905 generators it should be acknowledged that the overly dissipative nature of the
 906 Smagorinsky model may significantly alter the comparison performed above
 907 between the computational results and the experimental data. It is therefore
 908 proposed in this subsection to analyze the different turbulence generators in
 909 conjunction with another subgrid-scale closure.

910 In practice, many solutions have been proposed to remedy the excessive
 911 dissipation of the standard Smagorinsky model. For instance, it has been com-
 912 bined with the similarity subgrid-scale model of Bardina et al. (1980) to obtain
 913 a *mixed* model, see Liu et al. (1994). Another solution consists in adjusting
 914 dynamically the Smagorinsky constant C_s to the flow conditions, following the
 915 procedure of Lilly (1992), *via* a double filtering in the physical space (Germano,
 916 1992). The computational results obtained with such a dynamic Smagorinsky
 917 closure are compared to experimental data in Figs. 19 and 20. From a general
 918 point of view, it must be recognized that the quality of the agreement between

919 computations and experiments is only slightly improved. However, the use of
 920 the dynamic procedure produces significantly better results for the level of fluc-
 921 tuations obtained at $x_1 = 7.8$, see Fig. 20.

Figure 19: Mean longitudinal velocity profiles obtained using the dynamic Smagorinsky model. (•): Experimental data (— · —) WN, (— —) DF, (· · ·) RFG and (—) SEM.

Figure 20: $\sqrt{R_{11}}$ stress tensor component profiles obtained using the dynamic Smagorinsky model. (•): Experimental data (— · —) WN, (— —) DF, (· · ·) RFG and (—) SEM.

922 7. Reactive flows simulations

923 Although there is already some literature available to describe the impor-
924 tance of realistic turbulent inflow data prescription on non-reactive flows, such
925 an analysis of the turbulent inflow data effects is much less common for turbu-
926 lent reactive flows. In this last section, a set of two-dimensional reactive flow
927 simulations is conducted to evidence such effects and then the paper ends with a
928 tri-dimensional numerical simulation performed with the RFG synthetic turbu-
929 lence model. The procedure followed here is identical to that adopted to impose
930 the turbulent boundary conditions in non-reactive flows, i.e., a set of numeri-
931 cal simulations was carried out in order to evaluate the effects of the different
932 methods for turbulent inflow generation: (i) superimposing white noise on the
933 mean velocity profile (WN model), using (ii) the DF method, (iii) the RFG
934 method and, finally, (iv) the SEM.

Table 2: Values for mean velocity profile retained for the simulation of reactive flows.

Duct	C_{in} [m/s]	h [m]	a [m]	γ_{in}
Main duct	55	0.02	0.08	6.0
Auxiliary duct	110	0.00	0.02	8.0

935 7.1. Two-dimensional numerical simulations

936 The computational domain is a three-dimensional box with dimensions $(800 \times$
937 $2 \times 100)$ mm³. It is discretized with a mesh of $320 \times 1 \times 100$ control volumes
938 in the x_1 , x_2 and x_3 -direction, respectively. Periodicity and no-slip boundary
939 conditions are imposed along x_2 the x_3 -directions respectively. The compu-
940 tational domain is divided into 8 parallel regions. The other parameters re-
941 main the same as those retained for non-reactive cases. For the simulation
942 conducted with the white noise, a fluctuation level of 20 per cent is imposed on
943 the streamwise velocity component, while fluctuations of 10 per cent are set for
944 the cross stream velocity component. For the simulations performed with the
945 DF method of Klein et al. (2003) the filter support size is set to 10, while one

thousand (1,000) Fourier modes are used for the simulations based on the RFG method of Smirnov et al. (2001). Ten thousands (10k) eddies are considered in the simulation conducted with the Synthetic Eddy Method (SEM). Magre et al. (1988) have provided a large amount of experimental data gathered in the geometry previously used by Moreau and Boutier (1977) for different flow conditions. The mean velocity profile has the same shape as the one employed for the non-reactive flows, see Eq. (14). However, to be consistent with the measurements performed in reactive conditions by Magre et al. (1988), the mean velocity profile is parameterized with the values reported in Tab. (2).

To proceed with the mathematical modelling of the chemical source term, we retain a single step, global, and irreversible reaction that involves the progress variable, i.e., a normalized temperature defined by $c \equiv (T - T_u)/(T_b - T_u)$ where the subscripts u and b denote fresh reactants and fully burned gases conditions respectively. The corresponding chemical reaction rate is given by $S(c) = A_\alpha \rho \dot{S}$, where the pre-exponential constant can be calculated as $A_\alpha = \Lambda S_L^2 / [\alpha \exp(-\beta/\alpha)]$ and $\dot{S} = (1-c) \exp[-\beta(1-c)/(1-\alpha(1-c))]$, see Williams (1985). In the previous expressions, α denotes a normalized temperature factor $\alpha = (T_b - T_u)/T_b$ and the reduced activation energy is $\beta = \alpha(T_a/T_b)$, where $T_a = E_a/R$ is the activation temperature, E_a is the activation energy and R is the universal constant of gases. Here, we set $E_a = 8,000 J/mole$, which is a value representative of CH_4 -air combustion. The DVODE algorithm of Byrne and Dean (1993) is employed to perform the numerical integration of the chemical reaction rate.

The initial and boundary conditions for the mean value of the progress variable at $x_1^* = 0$, are set with the following hyperbolic profile,

$$\tilde{c}(x_3) = \frac{c_q + c_p}{2} + \frac{c_q - c_p}{2} \tanh\left(\frac{2h(x_3)}{\delta_m} - \frac{2h_p}{\delta_m}\right), \quad (15)$$

where, c_q and c_p are the mean values of the progress variable of the auxiliary burner ($c_q = 1$; $T_b = 2000$ K) and of the main duct ($c_p = 0$; $T_u = 560$ K), respectively. The quantity h_p is the height of auxiliary duct. Concerning the Monte Carlo simulation, 50 particles per control volume are used and the Mil-

stein scheme is employed for the numerical integration of the system of SDEs.

976

977 Figure (21) shows instantaneous fields of the chemical reaction progress vari-
 978 able $\tilde{c}$ and the filtered chemical reaction rate $\tilde{S}(c)$ for the present set of numerical
 979 simulations. The method of turbulent inflow data generation clearly influences
 980 the shear layer spreading rate as well as the position of the instantaneous fil-
 981 tered flame front. For instance, if we consider the subfigure (a) of Fig. 21, the
 982 longitudinal span of the turbulent flame front obtained with the white noise is
 983 larger than the one obtained using the other three methods.

Figure 21: Instantaneous fields of chemical reaction progress variable $\tilde{c}$ - top, and chemical reaction rate $\tilde{S}(c)$ - bottom. The subfigures (a), (b), (c), and (d) display results of simulations with the respective inlet boundary condition methods: WN, DF, RFG and SEM.

Concerning the influence of the inlet boundary condition, we observe in Fig. 22 that accounting for a turbulence spectrum always gives rise to a shorter and thicker flame brush. The length of the 2D flame brush, based on the location of the iso-line $\langle c \rangle = 0.9$ in the x_1 direction, is found to be 560 mm for the simulation carried out with the superimposition of a white noise, while for the DF, RFG and SEM methods the lengths are 543, 497 and 414 mm respectively.

Figure 22: Averaged fields of the progress variable - top, and chemical reaction rate $S(c)$ - bottom. The subfigures (a), (b), (c), and (d) are results of simulations with the respective inlet boundary condition methods: WN, DF, RFG and SEM.

Finally, an interesting point that can be evidenced from the present investigation is to determine how the choice of the method of generation of turbulent inflow data may affect the representation of the flame-turbulence interaction.

993 To this purpose, we recall the definition of the Damköhler number, $Da = \tau_t/\tau_c$,
 994 which is the ratio of the characteristic turbulent time scale, τ_t and the chemical
 995 time scale, τ_c . This number is one of the quantities that characterizes how tur-
 996 bulence interacts with chemical reactions. It should be noted that the different
 997 synthetic turbulence generators may lead to different Damköhler number values.

998 Indeed, the characteristic time of turbulence is strongly affected by the dif-
 999 ferent methods retained to generate inflow data. Considering the white noise
 1000 technique, we observed that the fluctuations lie in the range 1 – 20 m/s, whereas
 1001 using the DF, RFG and SEM methods, the maximum value of fluctuations down-
 1002 stream of the flame brush are about 60, 40 and 70 m/s respectively. Given the
 1003 grid size and the computational domain retained in the present study, which
 1004 provide a minimum length of the control volumes of 1 mm, the turbulent char-
 1005 acteristic times for the WN, DF, RFG and SEM methods are $50\ \mu s$, $16\ \mu s$,
 1006 $25\ \mu s$ and $14\ \mu s$, respectively. For the cases simulated in the present work, the
 1007 Damköhler number value is found to be 0.11 for the white noise. For the simula-
 1008 tions performed with the DF, RFG and SEM methods, the Damköhler number
 1009 is 0.033, 0.055 and 0.03, respectively which clearly confirms how the results of
 1010 turbulent reactive flow simulations may be sensitive to the methodology used
 1011 to generate synthetic turbulence at inlet boundary conditions.

1012 7.2. *Three-dimensional versus two-dimensional numerical simulations*

1013 The reactive numerical simulations that are reported herein have been per-
 1014 formed using the PDF closure presented in section 3.1. Large Eddy Simulations
 1015 should theoretically be performed in 3D, but the present reactive computations,
 1016 which do involve the resolution of the PDF transport equation with a Lagrangian
 1017 Monte-Carlo solver, remain quite expensive. This is the reason why we have
 1018 resorted to 2D simulations so as to evaluate the sensivity of the computational
 1019 results to the four inlet turbulence generators. However, it is quite relevant to
 1020 question the use and impact of the 2D approximation. This point is still under
 1021 investigation but, for one given inlet turbulence generator, a preliminary answer
 1022 is provided in this last section of the manuscript.

1023 The computational domain is now a three-dimensional box with dimensions
1024 $(800 \times 50 \times 100) \text{ mm}^3$, discretized with a mesh of $320 \times 50 \times 100$ control volumes in
1025 the x_1 , x_2 and x_3 -direction, respectively. The computational domain is divided
1026 into 256 parallel regions, each featuring 6250 control volumes. No-slip boundary
1027 conditions are imposed over x_2 and x_3 -direction while the Orlanski's advective
1028 boundary condition is again used at the outlet. The RFG model is retained to
1029 generate the turbulent inflow data.

Figure 23: Instantaneous fields of the filtered chemical reaction rate $\tilde{S}(c)$ in s^{-1} .

1030 Figures 23 and 24 display the instantaneous fields of the filtered chemical
1031 reaction rate and filtered progress variable. Figure 25 illustrates the important
1032 flow acceleration that is induced by the thermal heat release. Combustion is
1033 initiated just downstream of the channel entrance and further develops along
1034 the channel length to reach an anchoring position at the upper channel wall
1035 at around $x_1 = 400 \text{ mm}$ downstream of the splitter plate, which is consistent
1036 with the data gathered from experimental investigations. The flame is subject to
1037 a large turbulence intensity and, as a consequence, the filtered flame structure
1038 appears to be strongly wrinkled by the large-scale turbulence. From a qualitative
1039 point of view, the filtered flame features a thickness of the order of centimeters.
1040 A similar order of magnitude was reported from the experimental observations of
1041 Magre et al. (1988). Nevertheless, it is important to emphasize that
1042 the LES results cannot be used to provide a statement about possible flamelet
1043 broadening. LES provides only space-filtered quantities, in such a manner that a
1044 direct comparison between numerical and experimental results can be performed

1045 in a time-averaged statistical sense only. Such a comparison is reported in Fig.
 1046 26.

Figure 24: Instantaneous fields of the filtered progress variable $\tilde{c}$ (bottom).

Figure 25: Instantaneous field of the $\tilde{u}_1$ filtered velocity component.

1047 Comparing the temperature profiles obtained numerically with the experi-
 1048 ment, it is possible to observe in Fig. 26 that a reasonable level of agreement is
 1049 achieved. From the comparison between 2D and 3D results with experiments,
 1050 it seems that the 2D approximation offers a rather satisfactory picture of the
 1051 average temperature field. At the very least, the 3D computational results does
 1052 not cast doubt on the representativeness of the 2D results. Finally, it should be
 1053 acknowledged that the limitations associated to the modeling of the chemical ki-
 1054 netics, i.e., global single-step chemistry, as well as the uncertainties that remain
 1055 in the closure of micro-mixing terms for premixed conditions (Mura et al., 2003;
 1056 Mura and Champion, 2009), suffice to explain the residual differences observed
 1057 between computational results and experimental data.

Figure 26: Mean temperature profile at (a): $x_1^* = 8.4$ (top) and (b): $x_1^* = 24.4$ (bottom); • Experimental data; (—) 2D results; (- -) 3D results.

1058 8. Conclusion

1059 Large Eddy Simulations of both reactive and non-reactive turbulent chan-
 1060 nel flows of methane/air mixtures have been conducted with special emphasis
 1061 placed on the influence of turbulent inlet Boundary Conditions. The analysis
 1062 undoubtedly confirms the sensitivity of the obtained results to the choice of the
 1063 synthetic turbulence generator retained at the inlet of the computational do-
 1064 main. For the sake of completeness this sensitivity study is conducted for four

1065 distinct turbulent inflow conditions including *white noise* (WN), *digital filter*
 1066 (DF) by Klein et al. (2003), *random flow generator* (RFG) by Smirnov et al.
 1067 (2001), and *synthetic eddy model* (SEM) of Jarrin et al. (2009). The capability
 1068 of each method to reproduce a prescribed Reynolds stress tensor at the inlet
 1069 BC is first evaluated quantitatively. The energy spectrum associated with the
 1070 corresponding fluctuating velocity field are also examined. This analysis pro-
 1071 vides some interesting bases to explain the behavior that is observed when the
 1072 synthetic turbulence generators are used to perform three-dimensional LES of
 1073 high-speed mixing layers. The computational results of the corresponding LES
 1074 are investigated in details and the quality of the agreement with experimental
 1075 data is found to be significantly improved by resorting to elaborated synthetic
 1076 turbulence generators that accounts for the large scale dynamics and coherence.
 1077 The results obtained for reactive flow conditions also clearly emphasize the in-
 1078 fluence of the retained model on the chemical rate statistics, which confirms
 1079 the importance of this issue for the LES of turbulent reactive flows. From the
 1080 computational cost point of view, the DF, RFG and SEM methods obviously
 1081 require longer CPU time than the WN. For the present applications, the addi-
 1082 tional CPU costs lie between 35 per cent for the method of Smirnov et al. (2001),
 1083 and 55 per cent for the method of Klein et al. (2003), which remains moderate
 1084 considering the potential improvements that may be obtained from their use.
 1085 Finally, in the light of the obtained results, the RFG and SEM frameworks are
 1086 found to offer the best compromises between computational costs and physical
 1087 relevance.

1088

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