

Cold flow characteristics of a novel bluff body hydrogen burner

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Abstract

The cold flow characteristics of a novel partial premixed bluff body (PPBB) low NO_x burner, capable of operating with hydrogen as well as methane-hydrogen blends, were investigated numerically. The PPBB burner features a frustum shaped conical bluff body generating a flame stabilizing recirculation zone. Fuel is partially premixed via jets in an accelerating cross-flow. Steady-state and transient non-reacting simulations using five different turbulence models, i.e. standard k- ϵ , realizable k- ϵ , shear stress transport (SST) k- ω , stress-blended eddy simulation (SBES) and large eddy simulation (LES), were conducted. The simulations were validated against particle image velocimetry (PIV) measurements of an unconfined non-reacting flow. All turbulent models were able to predict the recirculation zone length in good agreement with the experimental data. However, only scale resolving simulations could reproduce velocity magnitudes with sufficient accuracy. Time averaged and instantaneous results from the scale resolving simulation were

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analysed in order to investigate flow characteristics that are special about the PPBB burner design and of relevance for the combustion process. Two different burner configurations were studied and their effects on the flow field were examined. The recirculation zone volume as well as the entrainment into the wall jet around the bluff body were found to correlate with the elevation of the bluff body relative to the burner throat. Both of these parameters are expected to have a strong impact on the overall NO_x emission, since the near burner region is typically one of the main contributors to the NO_x formation. *Keywords:* bluff body flow, low NO_x burner, CFD simulations, turbulence modelling, stress-blended eddy simulation, conical wall jet

1. Introduction

Combustion of hydrogen and hydrogen-rich synthetic gaseous fuels, such as syngas have received increased attention in the context of climate change and the urgent need for alternative fuels [1, 2, 3]. The use of syngas is particularly attractive when obtained by gasification of coal, waste or CO_2 -neutral biomass feedstock. In case of steam gasification, it is possible to combine the process with a subsequent water-gas shift reaction, in which CO and H_2O are converted to H_2 and CO_2 . The CO_2 can then be captured and stored. This combined process is referred to as pre-combustion carbon capture and storage (CCS). Benefits of pre-combustion CCS are the maximisation of the hydrogen level and the high relative concentration of the carbon species as CO_2 [4, 5]. Although the combustion of hydrogen in air emits theoretically only water, the high reactivity and elevated combustion temperature generate harmful and regulated nitrogen oxides (NO_x), that to date, no com-

15 mercial burner can mitigate easily. Hence, transitioning from natural gas to
16 hydrogen and hydrogen-rich combustion comprises a trade-off between re-
17 duced CO₂ emissions and increased NO_x emissions. In order to mitigate this
18 undesired effect, low NO_x combustion concepts need to be developed, while
19 keeping the required fuel flexibility in mind.

20 Different techniques have been established in the industry to reduce NO_x
21 emissions from combustion processes. They can be categorized into four
22 groups: pre-treatment, combustion modification, process modification (such
23 as the modification of a gas turbine cycle [6]) and post-treatment [7]. A key
24 benefit of syngas is its wide flexibility in fuel sources [8]. However, this and
25 in particular different processing techniques imply a significant variation in
26 relative composition of syngas [9, 10], which makes pre-treatment challenging.
27 Most post-treatment methods on the other hand are relatively simple to
28 implement, but they represent expensive add-on costs and are not benefiting
29 the combustion process in any way [7]. The U.S. Environmental Protection
30 Agency (EPA) provides an overview on the total effective NO_x reduction
31 and the cost effectiveness of different control techniques [11]. The report
32 concludes that low NO_x and ultra low NO_x burner on its own have the best
33 cost effectiveness. While the lowest NO_x levels are achieved by a combination
34 of low NO_x burners and selective catalytic reduction (SCR). Hence, there is
35 a strong incentive to develop low NO_x burners for both standalone as well as
36 combined applications.

37 Low NO_x burners can utilize different design features to minimize NO_x
38 emissions. A discussion on several of these designs can for example be found
39 in previous studies [1, 9]. However, for the development of low NO_x burners

40 that can cope with variable fuel compositions and potentially high hydrogen
41 concentration special care needs to be taken, especially of combustion sta-
42 bility. Hydrogen has a unique impact on the behaviour of fuel mixtures due
43 to its significantly different transport properties and flame speed compared
44 to other gaseous fuels [12]. Several studies have investigated the non-linear
45 dependence of flame properties (e.g. flashback and lean blowout) on the hy-
46 drogen concentration [13, 14, 15]. Due to the wider flammability limits, low
47 levels of hydrogen can extend the lean stability limits of burners [16]. How-
48 ever, higher levels of hydrogen decrease the stability range, as a result of the
49 increased probability of flashbacks [13].

50 One of the most common designs for low NO_x gas burners is the premixed
51 swirl burner. However, such burners are particularly prone to flashbacks at
52 elevated hydrogen concentrations [17]. This is attributed to the premixing
53 as well as the potential for combustion induced vortex breakdown (CIVB),
54 which is related to the interaction of heat release and swirling flows [9, 18, 19].
55 In order to avoid these issues associated with premixed swirl burners, Span-
56 gelo et al. [20] developed and patented a novel partially premixed bluff body
57 burner (PPBB burner) that aims to ensure stable combustion with low NO_x
58 emissions across a wide range of hydrogen concentrations. The PPBB burner
59 combines advanced mixing techniques with burner generated internal flue gas
60 recirculation (IFGR), which is sometimes referred to as furnace gas recircu-
61 lation. A more detailed description of the PPBB burner design features is
62 given in section 2.

63 The PPBB burner has been investigated experimentally by Dutka et al.
64 and has proven good emission performance at laboratory scale [21, 22]. How-

65 ever, the scalability of the system is not yet well understood. For a successful
66 scaling of the burner to larger dimensions and practical applications it is nec-
67 essary to obtain a deeper understanding of the burner flow characteristics and
68 their changes at different scales. The conducted experimental campaigns have
69 been limited to the analysis of the flow field in a defined 2D observation win-
70 dow downstream of the bluff body as well as global emission measurements
71 for NO_x , O_2 , CO and CO_2 . One of the main objectives for the present study
72 is therefore to extend the investigated parameters by applying computational
73 fluid dynamic (CFD) simulations, which allow to get a broader picture of the
74 flow characteristics. In the context of scaling the main requirement for CFD
75 simulations is to adequately represent qualitative trends depending on the
76 burner scale. However, simulating the entire complexity of hydrogen combus-
77 tion in a challenging geometry, including chemical reactions, different species
78 properties, radiation, etc. involves the use of several submodels in addition
79 to solving the equations describing the turbulent flow field. Hence, it is am-
80 biguous to quantify uncertainties attributed to individual submodels. Thus
81 the complexity of such a simulation needs to be increased gradually. The
82 scope of the present study was therefore limited to the modelling of the non
83 reacting air flow, which dominates the burner aerodynamics. This approach
84 allows a clear distinction between aerodynamic and combustion driven effects
85 and builds a solid foundation for future investigations with increased model
86 complexity and focus on different burner scales.

87 By excluding any chemical reactions from the flow it was possible to
88 validate the turbulence model without the additional uncertainty that de-
89 rives from the various submodels related to combustion. Different turbulence

90 models were employed to identify the model requirements for an adequate de-
91 scription of the major burner characteristics. The applied turbulence models
92 ranged from two equation RANS models, that model the whole turbulence
93 spectrum, to LES simulations which resolve the large scales and model only
94 the subgrid scales. A comprehensive comparison was made between well-
95 known models such as the standard k- ϵ model and a novel stress-blended
96 eddy simulation (SBES) model, which has been recently developed by the
97 ANSYS[®] turbulence team [23, 24]. The SBES model represents a compro-
98 mise between RANS and LES models. It resolves large scale turbulence only
99 away from walls, while modelling the entire turbulence spectrum close to
100 walls. A more detailed descriptions of the underlying numerics of the SBES
101 model is provided in section 3. All conducted numerical simulations were
102 validated against the measurements obtained by Dutka et al. [25, 26].

103 **2. The PPBB burner**

104 The PPBB burner is designed for furnaces and boilers, operating at low
105 pressure. Its main components consist of a cylindrical lance, holding a con-
106 ical frustum shaped bluff body mounted concentrically, within a cylindrical
107 housing (see figure 1). The bluff buddy is partially retracted into the housing
108 forming a converging segment in which the narrowest cross-section is referred
109 to as burner throat. The bluff body holds eight primary fuel ports located
110 upstream of the throat and four secondary fuel ports downstream of the
111 throat. Note that the secondary fuel ports are offset from the primary fuel
112 ports in tangential direction (i.e., they are located "between" primary fuel
113 ports). The laboratory scale burner operates at a nominal thermal load of

114 10 kW.

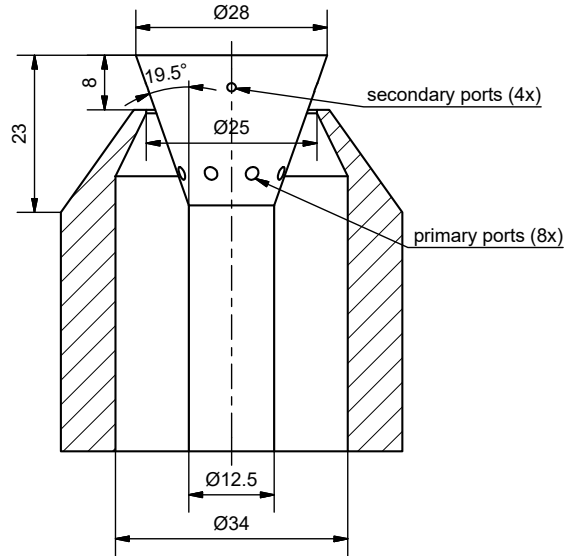


Figure 1: Schematic of the PPBB burner (dimensions in mm).

115 Figure 2 illustrates the flow pattern generated by the PPBB burner. Air
116 is provided through the annular duct formed by the lance and burner housing.
117 The majority of fuel (70% of the total fuel mass flow) is provided through
118 the primary fuel ports, located in the converging section of the burner, where
119 it is mixed in the accelerating cross flow. This configuration allows for rapid
120 mixing and avoids ignitable unburned mixture in low axial velocity regions,
121 which potentially could lead to flashback in the core flow, a well known
122 phenomena as described by Plee and Mellor [27]. Furthermore, the acceler-
123 ating flow ensures thin boundary layers, preventing flame back propagation
124 within the boundary layer itself. Flashback in the boundary layer has been
125 extensively studied for conventional fuels such as pure methane [28, 29, 30]
126 and more recently also for syngas with different hydrogen concentrations

127 [31, 32, 33]. Lieuwen et al. [9] concludes: "Keeping the boundary layers as
128 thin as possible is an essential design criterion for syngas burners [...]"

129 The remaining 30% fuel mass flow is provided through the secondary fuel
130 ports downstream of the throat, which creates small regions of enriched mix-
131 ture downstream of the bluff body trailing edge. Dutka et al. [25] investi-
132 gated the effect of different secondary fuel fractions on flame stability and
133 NO_x emissions. The study showed that the impact of secondary fuel on the
134 burner performance is correlating strongly to the hydrogen concentration in
135 the fuel as well as the lance height (i.e., elevation of the bluff body trailing
136 edge in relation to the throat). The burner configurations assessed in the
137 present study (i.e., 8 mm and 16 mm lance height) have been found to pro-
138 vide optimal emission performance for the PPBB burner operating with pure
139 hydrogen and pure methane respectively [25].

140 Bluff body flame stabilization has been studied extensively, even though
141 it is less common than swirl flame stabilization. Recent studies of conical
142 bluff body stabilized flames have been conducted by Kariuki et al. [34, 35]
143 (unconfined), Andreini et al. [36] (confined) and Dawson et al. [37] (confined
144 and unconfined). A unique feature of the PPBB burner is, however, the
145 elevated position of the bluff body with regards to the burner throat (see
146 figure 1). Since the bluff body is not fully immersed, it is possible to realize
147 a minimum housing diameter that is smaller than the bluff body diameter
148 itself. This leads to a blockage ratio larger than 100%, where the blockage
149 ratio is defined as the ratio of bluff body cross section to minimum housing
150 cross section. The PPBB can therefore be characterized by a conical wall jet
151 flow around the bluff body. Only limited studies have investigated conical

152 wall jets [38, 39, 40]. Research activities are mainly focusing on plane, radial
 153 or cylindrical wall jets. The latter two can be seen as limiting cases of a
 154 conical wall jet for a half-angle of 90° and 0° respectively. The plane wall
 155 jet is in turn the limiting case for a cylindrical wall jet with infinite large
 156 radius. Sharma [38] found that the spread angle as well as the shape of the
 157 velocity profiles are independent of the cone half-angle. The decrease of the
 158 maximal jet velocity in flow direction is on the other hand depending on the
 159 half-angle. The velocity decreases faster with an increased half-angle.

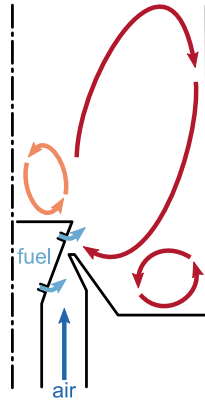


Figure 2: Illustration of the PPBB burner flow pattern. Primary and secondary fuel ports are drawn in the same plane for illustration purpose.

160 The elevated lance position is a crucial and unique feature of the PPBB
 161 burner for NO_x emission control and fuel flexibility. It allows entrainment of
 162 internal recirculated flue gas into the conical wall jet upstream of the flame
 163 anchor point (see figure 2). Recirculation of flue gas internally increases the
 164 overall efficiency compared to external flue gas recirculation. Understand-
 165 ing and controlling the amount of recirculated flue gas is therefore highly
 166 important.

167 **3. Numerical methods**

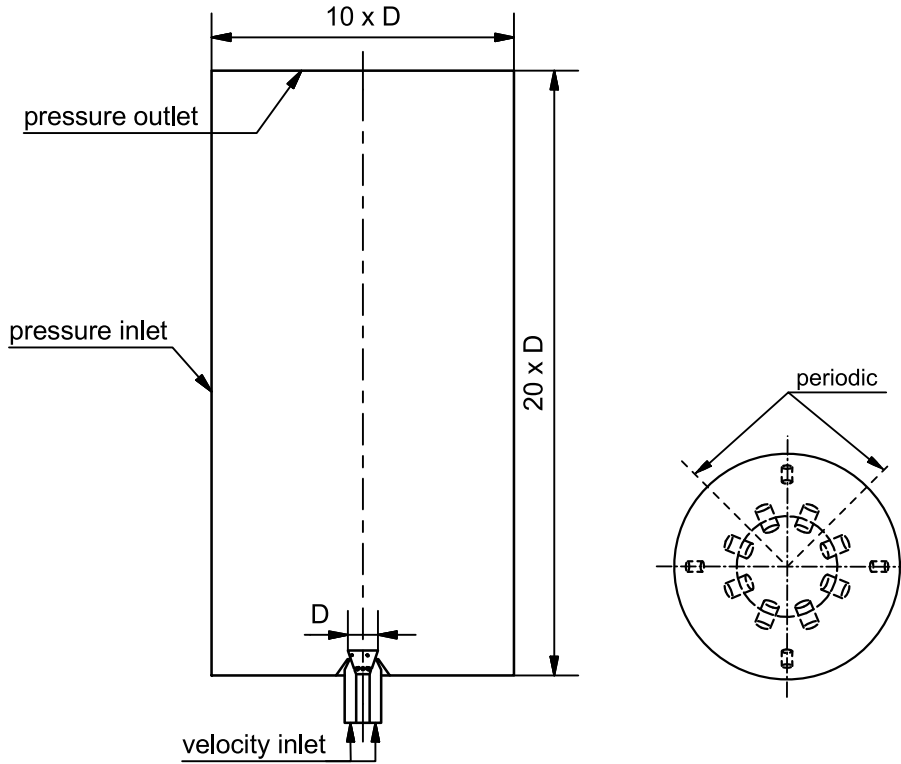
168 The PPBB burner was simulated using steady-state Reynolds averaged
169 (RANS) as well as transient scale resolving simulations employing ANSYS[®]
170 Academic Fluent, Release 18.1. All simulations were based on the assump-
171 tion of incompressible flow. The density was calculated based on the incom-
172 pressible ideal gas law based on the operational pressure (i.e., atmospheric
173 pressure for the PPBB burner). The highest velocities in the PPBB burner
174 (realized in the burner throat) are significant lower then the speed of sound
175 in air (i.e., $Ma \sim 0.15$) which justifies this assumption. Gravitational forces
176 were neglected.

177 The governing equations for the conservation of mass and momentum as
178 well as the transport equations for the respective turbulence model were dis-
179 cretised based on the finite volume method. A second order upwind scheme
180 [41] was used to discretise the convective terms of the RANS transport equa-
181 tions and a less dissipative bounded central difference scheme [42] was used
182 for the scale resolving simulations. The diffusive terms were discretised with
183 a second order central difference scheme. The transient simulations were
184 realized by use of a bounded second order implicit scheme. The SIMPLEC
185 algorithm [43] was applied for the pressure-velocity coupling in all steady
186 state simulations while a fractional-step method (FSM) [44, 45, 46, 47] in
187 conjunction with a non-iterative time advancement (NITA) was used for all
188 transient simulations. The transport equations were solved using a point im-
189 plicit (Gauss-Seidel) linear equation solver in conjunction with an algebraic
190 multigrid method [48]. ANSYS[®] Academic Fluent, Release 18.1. employs a
191 co-located scheme (i.e., pressure and velocity are both stored at the cell cen-

192 tres) which requires a pressure interpolation scheme to retrieve the pressure
193 at the cell faces. A second order central difference scheme was used for the
194 pressure interpolation. Gradients and derivatives were evaluated employing a
195 cell-based method (i.e., least squares cell based gradient evaluation), solving
196 the coefficient matrix by use of the Gram-Schmidt process [49].

197 All transient simulations were conducted on the full domain as shown in
198 figure 3. Different domain sizes were tested to ensure that the boundaries
199 were located sufficiently far from the burner. A quarter of the domain was
200 used for all RANS simulations, such that only two primary and one secondary
201 fuel port were included in the domain. The RANS simulations were realised
202 using periodic boundary conditions (see figure 3b). The applied boundary
203 conditions are shown in figure 3. A constant velocity, normal to the boundary,
204 of 4.0 m/s for the 8 mm lance height and 4.2 m/s for the 16 mm lance
205 height configuration was imposed at the velocity inlet, corresponding to the
206 experimental setup [25]. The turbulence kinetic energy at the velocity inlet
207 was calculated based on the turbulence intensity which was assumed to be
208 5% and a hydraulic diameter of 4 mm (corresponding to the largest hole
209 diameter in the perforated plate used to stabilize the flow, see figure 3.2 b
210 in [50]) was used to estimate the corresponding turbulence dissipation rate.
211 Atmospheric pressure was imposed at all open boundaries together with a
212 turbulent intensity of 5% and a turbulent viscosity ratio of 10 which were
213 used to calculate the corresponding turbulence kinetic energy and dissipation
214 rate. Flow entering the domain at the pressure outlet or flow leaving the
215 domain at the pressure inlet was defined as backflow. The direction of the
216 backflow was set to be normal to the boundary for both of the pressure

217 boundaries. A sensitivity study with varying turbulent boundary conditions
 218 showed negligible effect on the main flow features.



(a) Side view of the computational domain at 8 mm lance height.

(b) Top view of the burner lance indicating the location of the periodic boundaries (dashed lines).

Figure 3: Dimensions of the computational domain and boundary conditions. All unspecified boundaries are set to no-slip wall.

219 Five different turbulence modelling approaches, i.e. standard $k-\epsilon$ [51],
 220 realizable $k-\epsilon$ [52], SST $k-\omega$ [53], SBES [23, 24] and LES with the WALE
 221 subgrid model [54], were investigated. All RANS models were applied in
 222 steady state as well as unsteady (URANS) mode. The LES simulations have

223 been performed on the same numerical grid as the SBES simulations, hence
 224 under resolving the wall boundary layers. The SBES model represents a
 225 new paradigm of turbulence modelling. A further description of the model
 226 is therefore provided in the following paragraph. Descriptions of the other
 227 turbulence models can be found in the corresponding literature.

228 The SBES model is a RANS-LES hybrid model capable of switching
 229 rapidly from an underlying RANS model to an algebraic LES model. The
 230 SBES formulation is based on the the shielded detached eddy simulation
 231 (SDES) model, which aims to prevent grid-induced separation (one of the
 232 main shortcomings of detached eddy simulation models) by introducing an
 233 asymptotic shielding function, f_s and an alternative grid scale. The strong
 234 shielding of f_s allows the SBES formulation to blend existing RANS and LES
 235 models on the stress-level:

$$\tau_{ij}^{SBES} = f_s \cdot \tau_{ij}^{RANS} + (1 - f_s) \cdot \tau_{ij}^{LES} \quad (1)$$

236 where τ_{ij}^{RANS} is the RANS part and τ_{ij}^{LES} the LES part of the modelled stress
 237 tensor. If both, the RANS and the LES model, are eddy-viscosity models
 238 the formulation simplifies to:

$$\nu_t^{SBES} = f_s \cdot \nu_t^{RANS} + (1 - f_s) \cdot \nu_t^{LES}. \quad (2)$$

239 The SBES formulation is in this sense not a new turbulence model, but rather
 240 a novel way to blend two existing models. This approach allows therefore
 241 to combine different RANS and LES models. The SBES model has, to the
 242 authors knowledge, not yet been employed for studying advanced burner
 243 configurations such as the PPBB burner. The SBES simulations of the PPBB

244 burner were conducted by blending the SST-k- ω model in the RANS region
245 with the WALE subgrid model in the LES region.

246 The PPBB burner represents a complex geometry due to the arrangement
247 of its several fuel ports. It is challenging to represent such a geometry with a
248 structured hexahedral mesh. Several alternative mesh topologies (i.e., tetra-
249 hedral, polyhedral, cut-cell and tetrahedral/hexahedral hybrid mesh) were
250 tested in this study. Hybrid meshes utilize the flexibility of unstructured
251 meshes in complex areas of the fluid domain while maintaining the higher
252 accuracy of structured hexahedral meshes in simpler regions. However, they
253 are not as easily generated as fully unstructured meshes and extra attention
254 has to be given to the transition region between different mesh topologies
255 (i.e., from tetrahedral/polyhedral to hexahedral cells). Hybrid meshes are
256 therefore not ideal for the future up scaling of the PPBB burner, which
257 will require the generation of multiple different meshes. Cut-cell meshes on
258 the other hand can be generated using highly automated algorithms. They
259 are characterized by predominantly high quality hexahedral cells. However,
260 this comes at the cost of a few cells adjacent to the geometry with very
261 high skewness. These low quality cells led to slow convergence of the PPBB
262 burner simulations. Both tetrahedral and polyhedral meshes show a more
263 uniformly distributed mesh quality and can easily adapt to complex geome-
264 try. Polyhedral meshes achieve the same accuracy as tetrahedral meshes at
265 lower computational costs since they typically result in a significant lower
266 total cell count than tetrahedral meshes. An unstructured polyhedral mesh
267 with prism inflation layers at the walls was therefore found to be the most
268 suited mesh topology for simulating the PPBB burner (see figure 4).

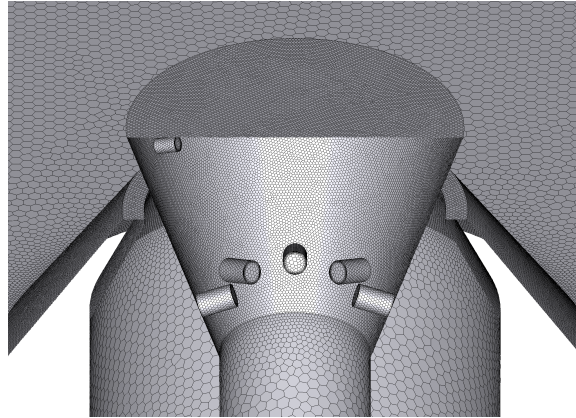


Figure 4: Half section view of the polyhedral surface mesh.

269 The mesh resolution was optimized for various flow regions by prescribing
270 a size field (i.e., location specific maximum cell sizes). An example of such
271 a size field can be seen in figure 5. A better representation of the transition
272 between different cell size regions can be seen in figure 4. The growth rate in
273 cell size was restricted to a maximum of 10% to ensure smooth transitions.
274 However, initial scale resolving simulations indicated that the relatively nar-
275 row refinement shown in figure 5 had a noticeable effect on the flow field for
276 the 8 mm lance height simulation. The refinement of the free shear layer
277 and recirculation zone was therefore extended to a cylindrical region with a
278 diameter of approximately two bluff body diameters and a height of 1.5 bluff
279 body diameters for the scale resolving simulation of the 8 mm lance height.
280 Mesh sensitivity simulations with different cell counts ranging from 2.9 M
281 to 8.2 M cells were conducted. The final scale resolving simulations were
282 realised with 4.0 M cells for the 16 mm configuration and 5.2 M cells for the
283 8 mm configuration. Boundary layer regions were resolved with values for
284 the dimensionless wall distance (y^+) close to unity. The warped-face gradi-

285 ent correction was employed to improve gradient accuracy for non planar cell
286 faces.

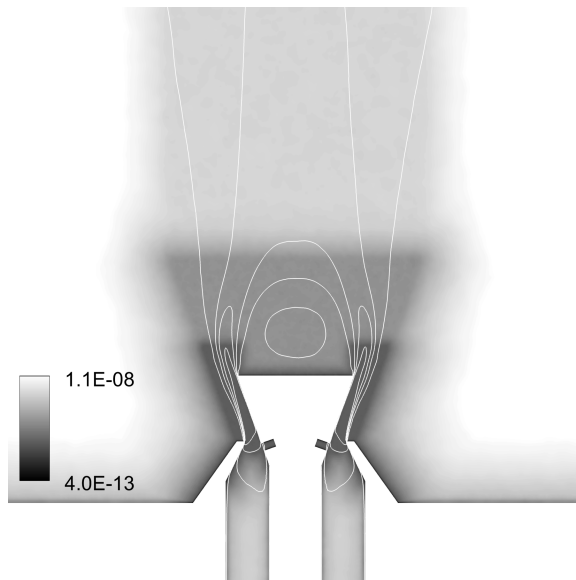


Figure 5: Cell volume with overlaid mean axial velocity iso-lines from the scale resolving 16 mm lance height simulation. Note an exponential colour scale is used for better readability.

287 4. Results

288 The results of the CFD based analysis are presented in three sections:
289 Reynolds averaged simulations (4.1), scale resolving simulations (4.2) and
290 the effect of different lance configurations (4.3). The first two sections are
291 dealing with the validation of the applied CFD models, while the last one
292 focuses on the alteration of the PPBB burner operational mode and its effect
293 on the flow field characteristics, especially in regions that have not been
294 accessible to PIV measurements.

295 *4.1. Reynolds averaged simulations*

296 Axial velocity profiles along the burner centreline were obtained from
297 RANS and URANS simulations using different turbulence models. A com-
298 parison of these profiles to PIV data acquired by Dutka et al. [25] is shown in
299 figure 6a and figure 6b respectively. All RANS simulations were able to pre-
300 dict the recirculation zone length. However, none of the applied models were
301 capable to capture the velocity magnitudes of the flow field with a reasonable
302 accuracy. All models were showing the same trend of over predicting veloc-
303 ities, especially within the recirculation zone. The SST $k-\omega$ model deviates
304 most from the experimental data as seen in figure 6a. However, it performed
305 better than the $k-\epsilon$ models in capturing the velocity decay in the developed
306 jet region downstream of the recirculation zone. Neither the standard, nor
307 the realizable $k-\epsilon$ model predicted the velocity decay correctly. The stan-
308 dard $k-\epsilon$ model was the only model that captured the maximal axial velocity
309 downstream of the recirculation zone.

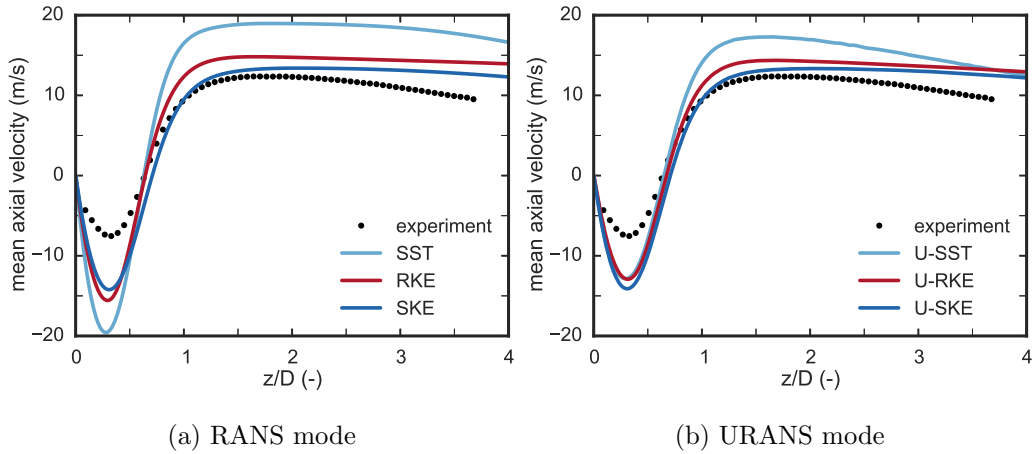


Figure 6: Mean axial velocity along the burner centreline for 8 mm lance height. Solid lines: standard k- ϵ (SKE), realizable k- ϵ (RKE) and SST k- ω (SST) simulations; dots: PIV measurement. Spatial coordinates are normalized by the bluff body diameter (D).

310 All three turbulence models were tested in URANS mode. The flow vari-
 311 ables were, depending on individual simulations, sampled over a time period
 312 of 1.5 to 2 seconds, after an initial build-up time of 0.2 to 0.5 seconds. The
 313 resulting time averaged axial velocity profiles along the burner centreline are
 314 shown in figure 6b. Switching to URANS mode did improve the performance
 315 of the SST k- ω model considerably. Both k- ϵ models performed compara-
 316 ble to the RANS simulations, with a slight improvement of the realizable
 317 k- ϵ model. The high dissipation of the standard k- ϵ model prohibited the
 318 development of unsteady flow structures.

319 The normalized recirculating mass flow rate is given in table 1, along with
 320 the normalized dimensions of the recirculation zone. Typically the recircu-
 321 lating mass flow rate is normalized by the mass flow rate at the trailing edge
 322 of the bluff body as suggested by Taylor and Whitelaw [55]. Since this region

323 was not captured by the PIV measurement, the inlet mass flow was used to
 324 normalize the recirculating mass flow rate. The recirculating mass flow rate
 325 measured by PIV was estimated based on the numerical integration of the
 326 axial velocity profile along the radius at the centre of the recirculation zone¹.
 327 All applied turbulence models were able to reproduce the recirculation zone
 328 dimensions. However, they severely over predicted the recirculating mass
 329 flow rate. The SST k- ω model in URANS mode led to the best results, but
 330 still over predicted the recirculating mass flow rate by a factor of 2-3.

Table 1: Recirculation zone length (L) and width (W) normalized by the bluff body diameter (D) and normalized recirculation mass flow rate ($\frac{\dot{m}_r}{\dot{m}}$) predicted by the two equation turbulence models.

		$\frac{L}{D}$ (-)	$\frac{W}{D}$ (-)	$\frac{\dot{m}_r}{\dot{m}}$ (-)
	experiment	0.64	0.70	0.36
RANS	SST k- ω	0.63	0.75	1.26
	realizable k- ϵ	0.64	0.75	1.15
	standard k- ϵ	0.71	0.74	1.12
URANS	SST k- ω	0.65	0.80	0.82
	realizable k- ϵ	0.67	0.80	1.08
	standard k- ϵ	0.71	0.78	0.97

¹The centre of the recirculation zone was defined by the axial coordinate of the highest recirculation velocity on the burner centreline.

331 *4.2. Scale resolving simulations*

332 An accurate description of velocity magnitudes and hence residence time
333 and recirculating mass flow rate in the recirculation zone is crucial for as-
334 sessing combustion emissions. Scale resolved simulations were conducted,
335 as the investigated RANS turbulence models performed poorly in this re-
336 gard. The complex geometry of the PPBB burner, especially in hydrogen
337 configuration (i.e., lance height of 8 mm) with large velocities in the narrow
338 (1.32 mm) throat, is computational demanding for scale resolving simula-
339 tions. The burner was therefore initially simulated in methane configuration
340 (i.e., lance height of 16 mm). This configuration allowed a finer spatial and
341 temporal resolution at lower numerical costs due to the wider throat opening
342 and lower flow velocities. Moreover, the variation of the lance height made a
343 qualitative assessment of its impact on the flow field accessible. The effect of
344 varying the lance height on the flow field (i.e., change of air entrainment and
345 recirculation zone length) is expected to be similar in the non-reacting and
346 reacting flow configuration, even though absolute values will be different for
347 these two scenarios. Experimental observations made by Dutka et al. [25]
348 support this assumption.

349 *4.2.1. Lance height 16 mm*

350 Figure 7a shows the comparison of the mean axial velocity measured ex-
351 perimentally (left) and the mean axial velocity simulated using the SBES
352 turbulence model (right). The velocity field of the SBES simulations was
353 in good agreement with the PIV measurements. The simulation displayed
354 slightly lower velocities in the centre of the flow and higher velocities in the
355 shear layer flow. Note that the velocity field measured by PIV appears dis-

356 torted close to the borders of the contour plot. This is attributed to the
357 limited number neighbouring interrogation windows at the borders. The
358 symmetry axis of the measured flow field is furthermore tilted by approxi-
359 mately 4° (see figure 7b). This was likely related to the difficulty of achieving
360 perfect symmetry in an experimental set-up. Asymmetry can be caused by
361 uneven air supply or centring inaccuracies of the lance. Small deviations in
362 the alignment of lance and housing axis have a strong influence on the sym-
363 metry of the throat width due to the relatively large distance between the
364 lance mounting point and the throat. Besides, flow field with recirculation
365 are inherently hydrodynamically unstable.

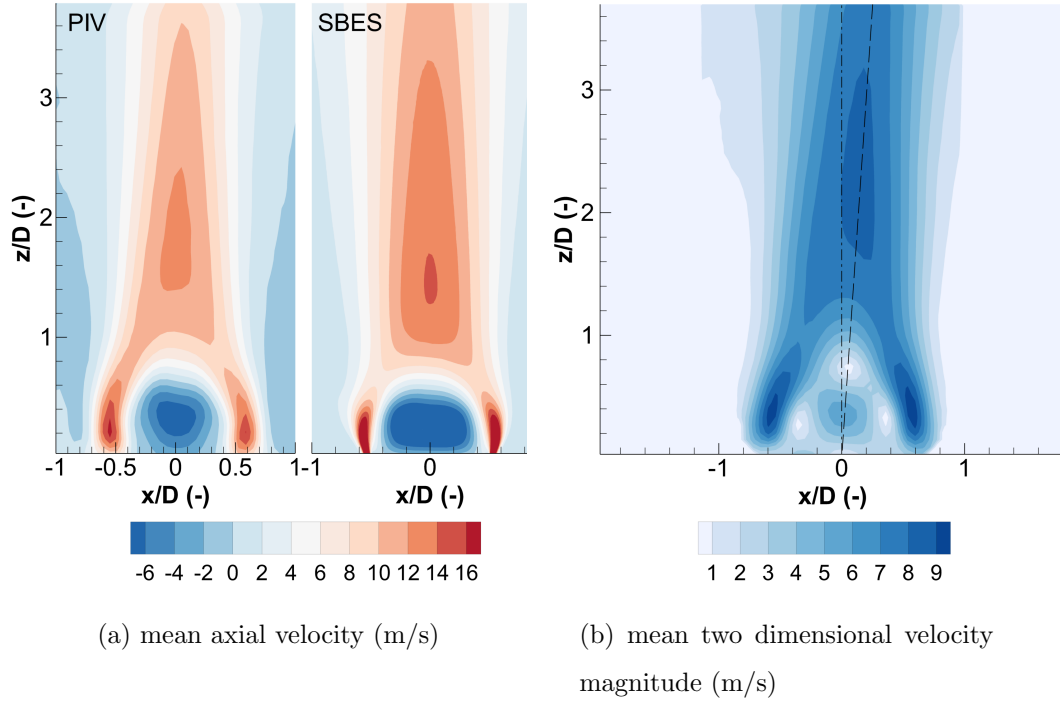


Figure 7: a) Mean axial velocity from PIV measurement (left) and SBES simulation (right). b) Measured two dimensional mean velocity magnitude. The flow symmetry axis (dashed line) is tilted by $\sim 4^\circ$ from the burner centreline (dash dotted).

366 Figure 8 shows the instantaneous visualisation of the iso-surface of the
 367 Q-criterion (which defines turbulent eddies as regions where the irrotational
 368 straining is small compared to the vorticity [56]) coloured by the SBES blend-
 369 ing function. It can be seen that the SBES model was able to shift quickly
 370 to LES mode (blue) outside the wall boundaries while structures close to the
 371 wall are in RANS mode (red). The model resolved small three-dimensional
 372 turbulent structures, which are visible in the recirculation zone.

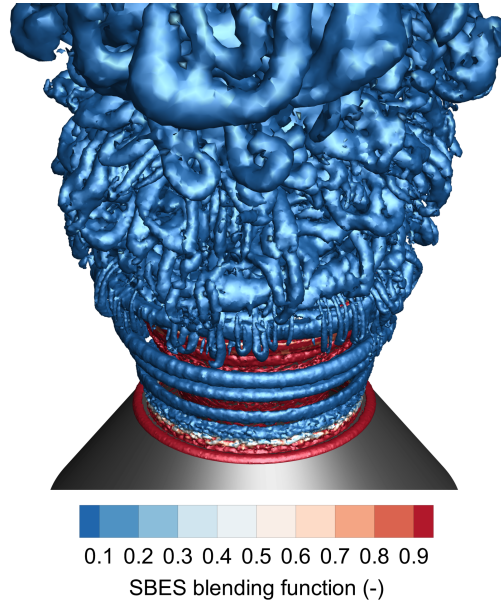


Figure 8: Q-criterion (10^4 s^{-2}) iso-surface coloured by the SBES blending function (where a value of 1 means RANS and a value of 0 means LES mode) from the 16 mm lance height simulation.

373 In figure 9 the velocity was corrected for the tilt of the flow field. The dots
 374 show the velocity along the symmetry axis of the flow, while the diamonds
 375 show the uncorrected velocity along the centreline of the burner. It is not pos-
 376 sible to identify or correct for tilting of the flow field outside of the 2D plane
 377 covered by the PIV measurement. Hence, the observed tilt in the xz -plane is
 378 indicating the failure margin that can be expected for alignment deviations
 379 in the experimental set-up. However, the impact of it is less noticeable closer
 380 to the bluff body and can be neglected within the recirculation zone. The
 381 SBES and LES simulations, using the WALE subgrid model, showed almost
 382 identical results along the burner centreline (see figure 9). Both were in good
 383 agreement with the experimental data. The velocity magnitude were slightly

384 under predicted by both modelling approaches. The difference between mea-
 385 sured and simulated recirculating mass flow rate as well as recirculation zone
 386 length were below 10% for both simulations (see table 2).

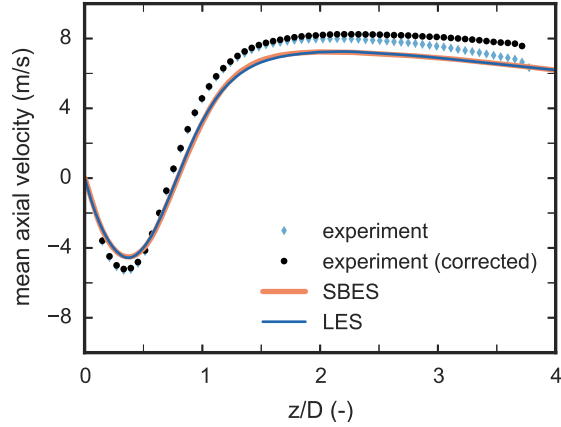


Figure 9: Mean axial velocity at 16 mm lance height. Bold red line: SBES simulation; blue line: LES simulation; diamonds: PIV measurement along burner centreline; dots: PIV measurement adjusted for $\sim 4^\circ$ tilt of the mean flow field (see figure 7b).

Table 2: Size of recirculation zone and recirculation mass flow rate for 16 mm lance height.

	$\frac{L}{D}$ (-)	$\frac{W}{D}$ (-)	$\frac{\dot{m}_r}{\dot{m}}$ (-)
PIV	0.73	0.71	0.26
SBES	0.79	0.81	0.28
LES	0.78	0.86	0.27

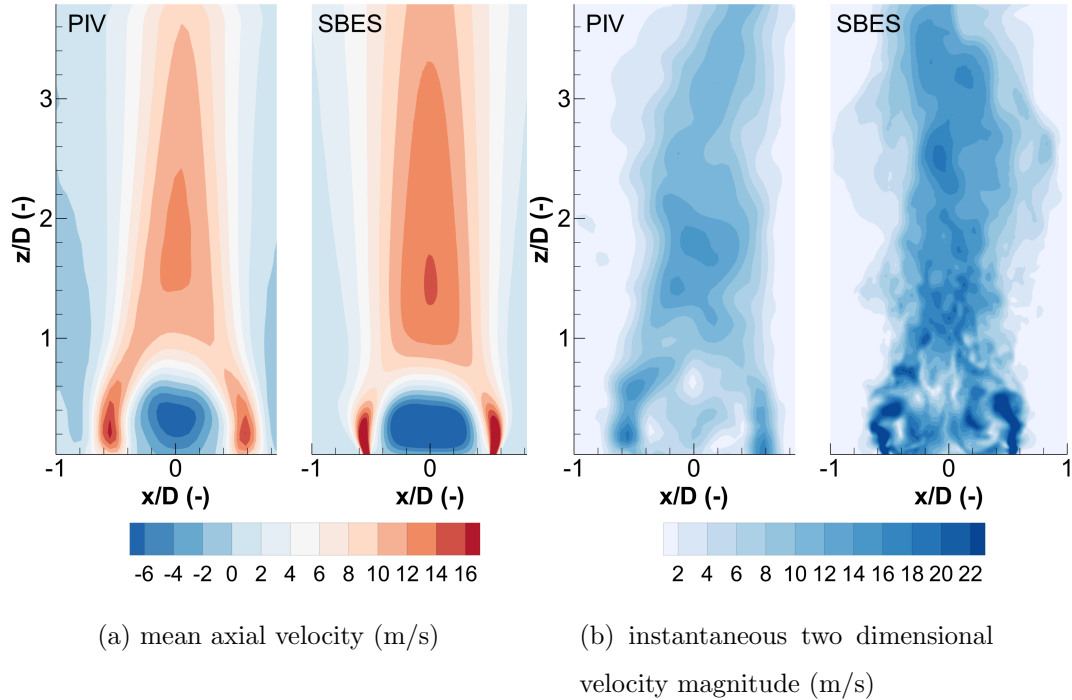


Figure 10: Comparison of mean and instantaneous velocity fields from PIV (left in the sub-figures) and SBES simulation (right in the sub-figures)

388 The measured flow field for 8 mm lance height did not display the same
 389 tilted symmetry axis as previous seen for the 16 mm lance height case (see
 390 figure 10b left), even though some asymmetry attributed to the experimental
 391 set up was still apparent. Comparing instantaneous flow fields from PIV
 392 and SBES simulations (see figure 10a) shows the higher resolution in the
 393 CFD simulation which allows to visualize smaller turbulent structures. The
 394 SBES simulation and the LES simulation, using the WALE subgrid model,
 395 produced very similar results. Figure 11 shows a comparison between these
 396 two models and experimental data as well as data from the SST $k-\omega$ model

397 in URANS mode. The scale resolving simulation were able to capture the
 398 recirculation zone length as well as the velocity decay in the developed jet
 399 region reasonable well. The velocity magnitude were over predicted by the
 400 scale resolving simulations and the shape of the recirculation zone appeared
 401 not as spherical as in the PIV measurements. This was also reflected in the
 402 recirculating mass flow rate, which was significantly over predicted by the
 403 scale resolving simulations (see table 3).

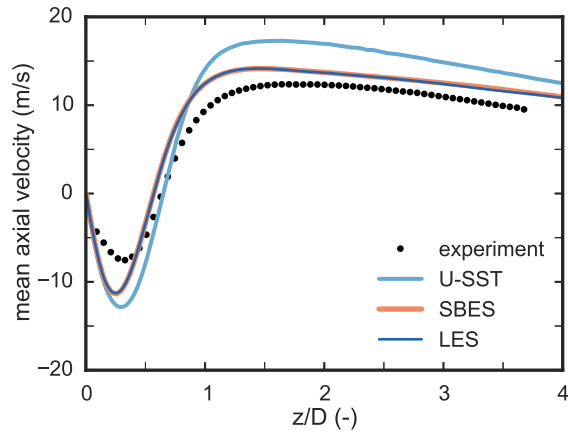


Figure 11: Mean axial velocity at 8 mm lance height. Light blue line: URANS SST $k-\omega$ simulation; bold red line: SBES simulation; thin dark blue line: LES simulation; dots: PIV measurement.

Table 3: Size of recirculation zone and recirculation mass flow rate for 8 mm lance height.

	$\frac{L}{D}$ (-)	$\frac{W}{D}$ (-)	$\frac{\dot{m}_r}{\dot{m}}$ (-)
PIV	0.64	0.70	0.36
SBES	0.57	0.80	1.56
LES	0.57	0.80	1.35

404 *4.3. Effect of different lance configurations*

405 Varying the lance height to adapt the PPBB burner to different fuel
406 compositions affects the opening of the throat, the length of the wall jet
407 region and the relative position of the fuel ports to the housing which leads
408 to a different momentum ratio of the jet in cross flow configuration of the fuel
409 injection. Extending the lance height increases the length of the recirculation
410 zone and decreases the recirculating mass flow rate. This effect was observed
411 in both the experiments and scale resolving simulations. The smaller throat
412 opening of the 8 mm configuration led to higher velocities in the free shear
413 layer downstream of the bluff body even though the air mass flow rate was
414 slightly lower than that for the 16 mm configuration (see figure 12). The
415 simulation of the 16 mm configuration under predicted the shear layer spread
416 compared to the experimental data more than the simulation of the 8 mm
417 configuration. However, the centre region of the flow was better reproduced
418 in the 16 mm simulation.

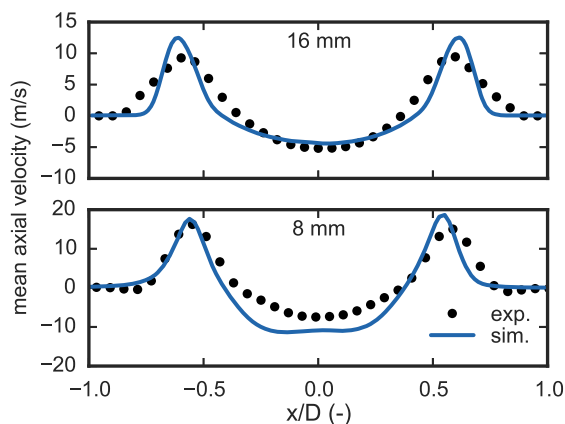


Figure 12: Axial velocity profile along the burner x-axis obtained from PIV (dots) and LES simulations (solid line) at 0.3 bluff body diameters downstream of the bluff body trailing edge.

419 The region close to the bluff body wall was not accessible by the con-
 420 ducted PIV measurements. Time averaged data of the wall jet was therefore
 421 obtained from the LES simulations for 8 mm and 16 mm lance height to give
 422 new insight into the flow structure in this region. Figure 13 shows a set of
 423 normalized velocity profiles close to the wall at various positions in flow direc-
 424 tion between throat and bluff body trailing edge. The velocity is decomposed
 425 into a component parallel to the wall (u_w) and a component perpendicular
 426 to the wall (v_w). The velocity is normalized by the maximum velocity in flow
 427 direction (u_{max}) and the wall coordinate (y_w) is normalized by the wall jet
 428 half-width ($y_{1/2}$) which is the cross-stream distance corresponding to half of
 429 the maximum velocity. The coordinate in flow direction (x_w) is normalized
 430 by minimum throat width (δ_{throat}). The velocity in the throat ($x_w/\delta_{throat}=0$)
 431 contains a noticeable velocity component towards the bluff body wall caused
 432 by the converging burner housing. This component decays in flow direction.

433 However, the velocity profiles do not reach self-similarity. A similar trend
 434 can be seen in figure 14a for the simulation of 8 mm lance height. However,
 435 at $x_w/\delta_{\text{throat}}=3.1$ the profiles start to collapse in the outer layer as seen in
 436 figure 14b.

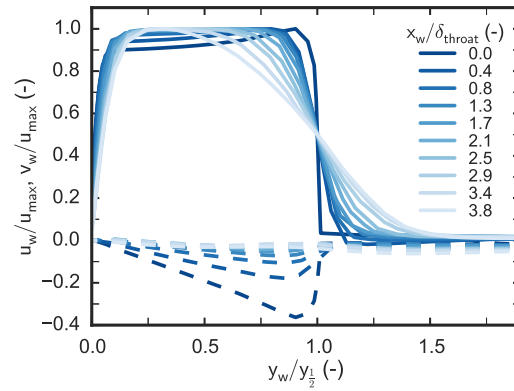


Figure 13: Normalized velocity profiles in the wall jet region obtained from LES simulations of 16 mm lance height. (solid lines) velocity component parallel to wall, (dashed lines) velocity component perpendicular to the wall.

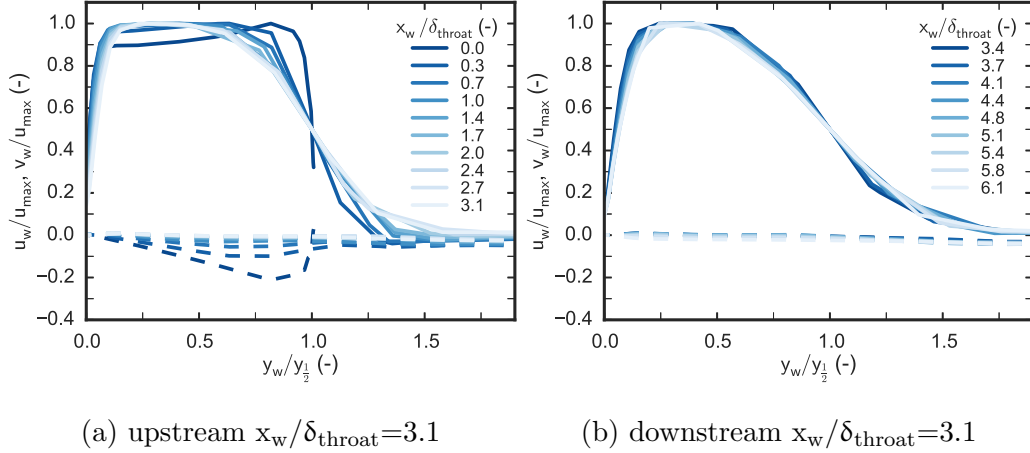


Figure 14: Normalized velocity profiles in the wall jet region obtained from LES simulations of 8 mm lance height. (solid lines) velocity component parallel to wall, (dashed lines) velocity component perpendicular to the wall.

437 The wall jet velocity and width at the bluff body trailing edge are impor-
 438 tant as they affect the recirculation zone. Figure 15 shows the decay of the
 439 maximum jet velocity and the jet spreading rate represented by the varia-
 440 tion of the half-width $y_{1/2}$. Increasing the lance height increases the throat
 441 opening as well. The normalized length of the wall jet in flow direction is
 442 therefore shorter for the 16 mm configuration compared to the 8 mm con-
 443 figuration. The jet half-width decreases for both lance heights initially and
 444 starts to increase again at $x_w/\delta_{throat}=3$. The decay of the maximum veloc-
 445 ity in flow direction shows an opposite trend. The difference of the velocity
 446 profiles between the two burner configurations is, however, not found to be
 447 as significant as the difference in the spreading rate.

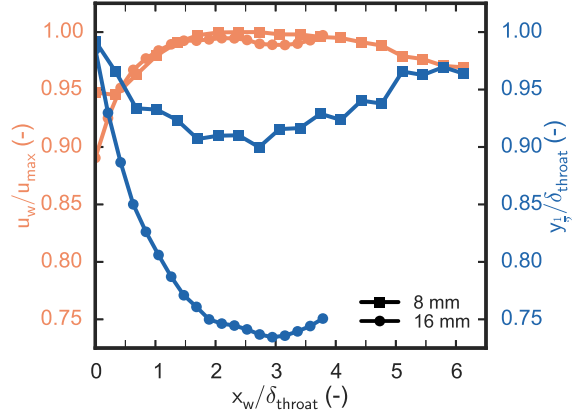


Figure 15: Decay of the maximum velocity (orange) and jet spreading rate (blue) for 8 mm lance height (squares) and 16 mm lance height (dots).

448 5. Discussion

449 The discussion is structured in three sections. Section 5.1 (turbulence
 450 model requirement) and section 5.2 (near wall treatment) discuss the re-
 451 quirements to the turbulence model. The latter one focuses on the two scale
 452 resolving turbulence models and their different near wall approaches only.
 453 Section 5.3 (PPBB burner flow characteristics) discusses the effect of differ-
 454 ent lance heights on the flow field, focusing mainly on regions that are likely
 455 to have a strong impact on the NO_x formation in a reacting flow. The lance
 456 height is one of the main burner parameters and its variation will affect the
 457 non-reacting and reacting configuration in a similar matter [25], which allows
 458 to draw qualitative conclusions based on the simulation of the non-reacting
 459 flow configuration.

460 *5.1. Turbulence model requirement*

461 All conducted RANS and URANS simulations over predicted the velocity
462 magnitude compared to the experimental data obtained from PIV measure-
463 ments. The high velocities in both the bluff body wake and recirculation
464 zone are a consequence of the over predicted velocity in the free shear layer
465 shedding from the bluff body trailing edge. Free shear layer flows are domi-
466 nated by different instability modes depending on the type of shear layer flow
467 (i.e., mixing layers, jets and wakes) which is challenging to accurately predict
468 with statistical averaged models using a single set of coefficients [57]. With
469 values for the coefficients that are appropriate to boundary-layer flows these
470 models typically predict two-dimensional flows, as for example a plane jet,
471 quite accurately. For axisymmetric flows with recirculation, however, effects
472 that are not existing in two dimensional flows (such as vortex stretching)
473 occur and can lead to large errors [58, 59].

474 This shortcoming of RANS turbulence models can be overcome by em-
475 ploying scale resolving simulations. Scale resolving simulations with an ap-
476 propriate spatial and temporal resolution are able to describe the flow char-
477 acteristics of the PPBB burner in good agreement with experimental data
478 as it was seen in the simulation of the 16 mm lance height configuration.
479 Furthermore it was shown that scale resolving simulation are superior to
480 RANS/URANS simulations, even with a lower relative resolution as seen in
481 the 8 mm lance height simulation. The difference in resolution between the
482 16 mm and the 8 mm simulation can be assessed by comparing the velocity
483 profiles in figure 13 with the profiles given in figure 14. The lower resolution
484 is furthermore leading to fluctuations of the normalized wall jet half-width

485 shown in figure 15. This is, however, due to the way the half-width is ob-
486 tained from a linear interpolation of the velocity profiles at the point $u_{\max}/2$.
487 Hence the resolution affects both the assessment of u_{\max} as well as the linear
488 interpolation, which magnifies the overall effect of different resolutions.

489 *5.2. Near wall treatment*

490 Typically it requires less effort to resolve the largest turbulence scales
491 in free shear flows compared to wall boundary layers, where the turbulence
492 length scale is very small compared to the boundary layer thickness. Apply-
493 ing LES models with under resolved wall boundary layers can, depending on
494 the flow configuration, led to worse results than employing a suitable RANS
495 model [23]. This motivated the development of hybrid models, such as the
496 SBES model, where large eddies are only resolved in the free flow, while the
497 wall boundary layer is covered by an URANS model. Hybrid models have
498 been applied to a variety of flow problems and have been proven to outper-
499 form RANS models for many applications [60, 61, 62]. The results of the
500 SBES simulations for both investigated lance heights confirm this general
501 trend.

502 The applied LES grid resolution in the wall boundary layer was far from
503 being sufficient to capture wall turbulence. However, LES and SBES sim-
504 ulation led to almost identical results. This indicates that the flow in the
505 PPBB burner is dominated by the free shear layer flow and the flow in the
506 recirculation zone, rather than the wall turbulence. The separation points
507 in the flow field are clear defined by the sharp trailing edges of the bluff
508 body and burner housing, which justifies the application of LES with under
509 resolved wall boundary layers over a hybrid model with proper boundary

510 layer treatment. Such a pragmatic approach has already been applied suc-
511 cessfully by others [63]. The main advantage of hybrid models over LES is
512 the lower computational cost due to a considerable coarser grid resolution
513 close to walls. Running LES and hybrid simulations on the same numerical
514 grid puts the hybrid model in the disadvantage of having to solve, typically
515 two, additional transport equations for the turbulence quantities. Hence, in
516 this specific case it can be beneficial to employ LES with an under resolved
517 wall regions.

518 *5.3. PPBB burner flow characteristics*

519 Flow conditions in recirculation zones created by bluff bodies or swirling
520 flow to stabilize turbulent flames (i.e., long enough residence times, high tem-
521 perature and oxygen concentration) do also promote NO_x production. The
522 recirculation zone has been identified as a major contributor to the overall
523 NO_x formation in bluff body and swirl burners respectively [64, 65]. The
524 NO_x formation depends on the volume of the recirculation zone, the temper-
525 ature and the concentration of oxygen and nitrogen, assuming that thermal
526 NO_x is the main contributor to the overall NO_x emission. The volume of
527 the recirculation zone scales typically proportional to cube of the burner
528 diameter [65]. The PIV measurements and CFD simulations of the PPBB
529 burner showed that a variation of the lance height affected the recirculation
530 zone length (the recirculation zone length shortened when the lance height
531 was decreased) while the width of the recirculation zone was less affected.
532 This indicates that the volume of the recirculation zone also correlates to the
533 lance height, which is consequently affecting the NO_x formation in the near-
534 burner region. The other important parameters for the NO_x formation in the

535 near-burner region, temperature and concentrations, are depending on the
536 dilution level [65]. Internal recirculated flue gas which is entrained into the
537 wall jet region of the PPBB burner will therefore affect these two parameters
538 and hence impact the NO_x formation. Quantifying this effect based on cold
539 flow simulations is not possible. However, the axial velocity profiles along
540 the x-coordinate at bluff body trailing edge elevation give an indication of
541 the entrainment as function of the lance height. Numerical integration of the
542 velocity profiles (see figures 13 and 14) showed that the wall jet in the 16 mm
543 configuration entrains 26% less than the wall jet in the 8 mm configuration.

544 **6. Conclusion**

545 In the present work, non-reacting CFD simulations of the PPBB burner
546 were conducted. Different turbulence models were investigated, ranging from
547 steady state RANS to scale resolving simulations, in order to identify the nu-
548 merical requirements for a reasonable accurate representation of the burners
549 main flow characteristics. The results evidence the need of scale resolving
550 simulations. RANS simulations over predicted velocity magnitude by a large
551 margin and were hence not able to describe the flow field adequately.

552 Scale resolving simulations with two different turbulence models were
553 carried out, the novel SBES model and LES simulations with the WALE
554 subgrid model. It was found that the SBES model is able to predict the
555 PPBB burner flow field in good agreement with experimental data. However,
556 conducting LES simulations on the same numerical grid and hence under
557 resolving the wall boundary layers led to almost identical results as the SBES
558 model. For the specific case of the PPBB burner, it is therefore advantageous

559 to use coarse LES simulations over SBES simulations in order to reduce the
560 overall computational costs.

561 The dimensions of the recirculation zone downstream of the bluff body
562 as well as the recirculating mass flow rate were quantified for two different
563 lance heights. The results indicate that the recirculation zone volume and the
564 recirculating mass flow rate scale proportional to the lance height. However,
565 more burner configurations need to be studied in order to further specify the
566 correlation between these parameters. In addition reacting flow simulations
567 are required to quantify the affect on the NO_x emissions from the burner.

568 The conical wall jet configuration is a feature special to the PPBB burner
569 and was analysed in detail. The velocity profiles in the wall jet region contain
570 a velocity component perpendicular to the wall, which is unusual for wall jets
571 investigated in the literature. This component decreases in flow direction and
572 for a lance height of 8 mm a self similar flow field is starting to establish at
573 $x_w/\delta_{\text{throat}}=3$. The wall jet configuration allows entrainment of internally
574 recirculated flue gas upstream of the bluff body trailing edge/flame anchor
575 point. It was found that increasing the lance height from 8 mm to 16 mm
576 results in a reduction of the wall jet entrainment by 26% (from 54% of the
577 inlet mass flow to 39%) which will lead to less dilution and hence affect the
578 overall NO_x formation. Further reacting flow simulations in a combustion
579 chamber need to be conducted in order to quantify the degree of dilution
580 due to the internal flue gas recirculation and the effect of a varying lance
581 height on it.

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